APPENDIX A

CHEMICAL-SPECIFIC DATA

DELISTING TECHNICAL SUPPORT DOCUMENT

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U.S. EPA
RCRA Delisting Team

APPENDIX A-1

CHEMICAL INFORMATION ON DRAS WASTE CONSTITUENTS

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Attachment

APPENDIX A-1

LIST OF VARIABLES AND COMPOUND-SPECIFIC PARAMETERS

Aquatic TRV	=	Ambient Water Quality Criteria (ì g/L)
B	=	Bunge constant (unitless)
BAF_{fish}	=	Bioaccumulation factor in fish (mg Chemical/kg FW tissue)/(mg Chemical/L total water column) OR (L water/kg FW tissue)
BCF_{fish}	=	Bioconcentration factor in fish (L/kg FW OR unitless)
D_a	=	Diffusivity of Chemical in air (cm^2/s)
D_w	=	Diffusivity of Chemical in water (cm^2/s)
H	=	Henry's law constant
Inhalation CSF	=	Inhalation cancer slope factor $(mg/kg\text{-}day)^{-1}$
Kd_s	=	Soil-water partition coefficient (L water/g soil OR cm^3 water/g soil)
Kd_{sw}	=	Suspended sediment-surface water partition coefficient (mL water/g bottom sediment OR cm^3 water/g bottom sediment)
K_{ow}	=	Octanol/water partitioning coefficient (mg Chemical/L octanol)/(mg Chemical/L octanol)—unitless
K_{oc}	=	Soil organic carbon-water partition coefficient (mL water/g soil)
$K_P{}^w$	=	Skin permeability constant in water (cm/hr)
MCL	=	National Primary Drinking Water Regulation (mg/L)
MW	=	Molecular weight of Chemical (g/mole)
Oral CSF	=	Oral cancer slope factor $(mg/kg\text{-}day)^{-1}$
RfC	=	Reference concentration (mg/m^3)
RfD	=	Reference dose (mg/kg/day)
Sol	=	Solubility of Chemical in water (mg Chemical/L water)
$\hat{o}$	=	Lag time (hr)
t^*	=	Time to skin permeability steady state (hr/event)
T_m	=	Melting point temperature (K)
V_p	=	Vapor pressure of Chemical (atm)

APPENDIX A-1

The following sections provide the methodology and rationale followed for the selection or development of compound-specific parameter values recommended by U.S. EPA OSW. Compound-specific values are provided for (1) physical and chemical properties, (2) fate-and-transport parameters, and (3) health benchmarks. A summary table of all compound-specific parameter values is provided at the end of this appendix, followed by individual parameter-value tables for each compound. The individual parameter-value tables cite sources for each parameter value.

A.1.1 COMPOUND NAME with CHEMICAL ABSTRACTS SERVICE (CAS) NUMBER

The Appendix A-1 Tables of waste constituents included in the Delisting Risk Assessment Software (DRAS) program are lists the chemicals by most common compound name. The CAS number provided in parenthesis is a unique number assigned to each compound in the table.

A.1.2 PHYSICAL AND CHEMICAL PROPERTIES

Molecular Weight (*MW*)

Molecular weight (*MW*) of a compound is defined as the sum of atomic weights of all atoms in the compound's molecule.

Organics and Metals For most organics (except PCDDs and PCDFs) and metals, *MW* values were obtained from the following:

- Budavari, S., M.J. O'Neil, A. Smith, and P.E. Heckelman. 1989. *The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals.* 11th Edition. Merck and Company, Inc. Rahway, New Jersey.

MW values not provided in Budavari, O'Neil, Smith, and Heckelman (1989) were obtained from the following document:

- Montgomery, J.H., and L.M. Welkom. 1991. *Groundwater Chemicals Desk Reference.* Lewis Publishers. Chelsea, Michigan.

Because Budavari, O'Neil, Smith, and Heckelman (1989) provides *MW* values for most of the compounds evaluated, it was used as the primary source to ensure consistency. *MW* values are based on the compound's formula; and, the values in Budavari, O'Neil, Smith, and Heckelman (1989) are the same as the values cited in several literature sources. *MW* values for most of the compounds in the primary guidance documents were also obtained from Budavari, O'Neil, Smith, and Heckelman (1989).

PCDDs and PCDFs *MW* values for PCDDs and PCDFs were obtained from U.S. EPA (1994a).

Mercuric Compounds *MW* values for mercury and mercuric chloride were obtained from Budavari and others (1989). *MW* value for methyl mercury was obtained from U.S. EPA (1997g).

Melting Point Temperature (T_m)

Melting point temperature (T_m) is the temperature of the compound (in degree Kelvin [K]) at which the solid state of the compound undergoes a phase change to a liquid phase. At ambient temperatures and at an atmospheric pressure of 1 atmosphere, compounds are either in a solid or liquid state.

Organics and Metals For most organics (except PCDDs and PCDFs) and metals, values for T_m were obtained from Budavari, O'Neil, Smith, and Heckelman (1989). T_m values not provided in Budavari, O'Neil, Smith, and Heckelman (1989) were obtained from Montgomery and Welkolm (1991).

Because Budavari, O'Neil, Smith, and Heckelman (1989) provides T_m values for most of the compounds evaluated, it was used as the primary source to ensure consistency. T_m values in Budavari, O'Neil, Smith, and Heckelman (1989) were generally within 2 to 3 degrees of the values provided in literature sources reviewed. T_m values for most compounds in the primary guidance documents were also obtained from Budavari, O'Neil, Smith, and Heckelman (1989).

PCDDs and PCDFs *Tm* values for PCDDs and PCDFs were obtained from U.S. EPA (1994a). U.S. EPA (1994a) provides T_m values for PCDDs and PCDFs, that were obtained from various literature sources.

Vapor Pressure (*Vp*) and Aqueous Solubility (*S*)

The vapor pressure (*Vp*) of a substance is defined as the pressure in atmospheres exerted by the vapor (gas) of a compound when it is under equilibrium conditions. It provides a semi-quantitative rate at which it will volatilize from soil and/or water. The aqueous solubility (*S*) of a compound is defined as the saturated concentration of the compound in water (mg chemical/L water) at a given temperature and pressure, usually at soil/water temperatures and atmospheric pressure (Montgomery and Welkom 1991).

Organics For most organics (except PCDDs and PCDFs), values for *Vp* and *S* were obtained from the following:

- U.S. EPA 1994b. *Draft Report Chemical Properties for Soil Screening Levels*. Prepared for the Office of Emergency and Remedial Response. Washington, DC. July 26.

U.S. EPA (1994b) provides measured, calculated, and estimated values for *Vp* and *S* that were obtained from various literature sources. *Vp* values in U.S. EPA (1994b) were generally either measured (at 20°C to 25°C) or calculated values obtained from various literature sources. U.S. EPA (1994b), however, provides values for *Vp* corrected to 25°C. U.S. EPA (1995a) states that, because the distribution of many of the parameters is skewed, the geometric mean or the median values were preferable to the arithmetic mean values. Therefore, when available geometric mean values were preferred over the arithmetic mean values.

In U.S. EPA (1994b), *S* values were either measured (at 20°C to 30°C) or calculated values obtained from various literature sources. Although *S* values were measured at temperatures ranging from 20°C to 30°C, U.S. EPA (1994b) states that *S* values were not corrected to 25°C, because the variability in solubilities measured at 20°C to 25°C was within the overall range of measured values.

U.S. EPA (1994b) is the preferred source, because (1) sources and the conditions at which each value was obtained are provided, and (2) values were provided to 2 significant figures. Also, U.S. EPA (1994b)

provides multiple *Vp* and *S* values for each compound from several different literature sources; providing a recent, more comprehensive compilation of reported literature values. *Vp* and *S* values from U.S. EPA (1994b) were generally consistent with those provided in U.S. EPA (1994e) and U.S. EPA (1995a).

When *Vp* and *S* values were not available in U.S. EPA (1994b), they were obtained from one of three sources, in the following order of preference:

1. U.S. EPA (1994e)

2. U.S. EPA (1995a); values from which were obtained from one of three sources:

    a. Mackay, D., W.Y. Shiu, and K.C. Ma. 1992. *Illustrated Handbook of Physical-Chemical Properties and Environmental fate for Organic Chemicals. Volume I - Monoaromatic Hydrocarbons, Chlorobenzenes, and PCBs. Volume II-Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins and Dibenzofurans. Volume III - Volatile Organic Chemicals.* Lewis Publishers. Boca Raton, Florida.

    b. Howard, P.H. 1989-1993. *Handbook of Environmental Fate and Exposure Data For Organic Chemicals. Volumes I: Large Production and Priority Pollutants (1989). Volume II: Solvents (1990). Volume III: Pesticides (1991). Volume IV: Solvents2 (1993)*. Lewis Publishers. Chelsea, Michigan.

    c. Other referenced literature sources, when values were not available in Mackay, Shiu, and Ma (1992) or Howard (1989-1993).

3. U.S. EPA. 1994f. *Superfund Chemical Data Matrix (SCDM).* Office of Emergency and Remedial Response. Washington, DC. June.

Vp and *S* values in U.S. EPA (1994e) were geometric mean values obtained from various literature sources. References specific to sources of values for each compound were provided in U.S. EPA (1994e) and were, therefore, preferred over U.S. EPA (1995a) values.

Most *Vp* and *S* values in U.S. EPA (1995a) were obtained from Mackay, Shiu, and Ma (1992) or Howard (1989-1993). Mackay, Shiu, and Ma (1992) and Howard (1989-1993) obtain the "best" values after evaluation of various literature sources.

Vp values in U.S. EPA (1994f) were obtained from various literature sources. *S* values in U.S. EPA (1994f) were the geometric mean of values obtained from various literature sources.

Mercuric Compounds Mercury is a relatively volatile compound. *Vp* and *S* values for elemental mercury were obtained from Budavari, O'Neil, Smith, and Heckelman (1989). *Vp* and *S* values for methyl mercury were not found in the literature.

Henry's Law Constant (*H*)

Henry's Law constant (*H*) is also referred to as the air-water partition coefficient, and is defined as the ratio of the partial pressure of a compound in air to the concentration of the compound in water at a given temperature under equilibrium conditions. Henry's Law constant values generally can be (1) calculated from the theoretical equation defining the constant, (2) measured, or (3) estimated from the compound structure. Experimental and estimated *H* values from literature reports, however, are (1) very temperature-dependent and difficult to measure, (2) generally obtained from various literature sources that use different experimental and estimation methods, and (3) available for only a limited number of compounds.

Organics For organics (excluding PCDDs and PCDFs), *H* values were calculated from the following theoretical equation (Lyman, Reehl, and Rosenblast 1982) for consistency, using recommended *MW, S,* and *Vp* values:

$$H = \frac{Vp \cdot MW}{S} \qquad \text{Equation A1-1}$$

H	=	Henry's Law constant (atm-m^3/mole)
Vp	=	Vapor pressure of Chemical (atm)
S	=	Solubility of Chemical in water (mg Chemical/L water)

The primary guidance documents also used theoretical Equation A-1-1 to calculate *H* values.

PCDDs and PCDFs *H* values for PCDDs and PCDFs are calculated values obtained from U.S. EPA (1994a).

Metals For all metals (except mercury), *H* is zero, because *Vp*—because of the nonvolatile nature of the metals—and *S* are assumed to be zero.

Mercuric Compounds *H* values for elemental mercury, and methyl mercury were obtained from U.S. EPA (1997g).

Diffusivity of Chemicals in Air (D_a) and Water (D_w)

Diffusivity or diffusion coefficients in air (D_a) and water (D_w) are used to calculate the liquid or gas phase transfer of a Chemical into a water body.

Organics For organics (except PCDDs and PCDFs), diffusivity values were obtained directly from the CHEMDAT8 model chemical properties database (Worksheet DATATWO.WK1):

- U.S. EPA. 1994d. *CHEM8—Compound Properties Estimation and Data*. Version 1.00. CHEMDAT8 Air Emissions Program. Prepared for Chemicals and Petroleum Branch, OAQPS. Research Triangle Park. North Carolina. November 18.

The U.S. EPA (1994c) database uses empirical correlations with compound density and molecular weight to calculate diffusivity values. For compounds not in the U.S. EPA (1994c) database, diffusivity values were obtained by using the WATER8 model correlation equations for air and water diffusivities:

- U.S. EPA. 1995d. *WATER8—Air Emissions Models Wastewater Treatment*. Version 4.0. OAQPS. Research Triangle Park. North Carolina. May 1.

U.S. EPA (1995c) database values were predicted by using chemical-structural relationships. Diffusivity values for all compounds in the U.S. EPA (1994c) and (1995c) databases were either predicted or estimated. The primary guidance documents also recommended U.S. EPA (1994c) and (1995c) database model values. More recent documents, including the following, also recommended these values:

- U.S. EPA. 1996. *Soil Screening Guidance: Technical Background Document and User's Guide*. Office of Solid Waste and Emergency Response. Washington, DC. EPA/540/R-95/128. May.

For diffusivity values that were not available in these databases, D_w and D_a values were calculated using the following equations cited and recommended for use in U.S. EPA (1997g):

$$D_{a,i} = \frac{1.9}{(MW_i)^{2/3}} \qquad \text{Equation A1-2a}$$

$$D_{w,i} = \frac{22\times10^{-5}}{(MW_i)^{2/3}} \qquad \text{Equation A1-2b}$$

U.S. EPA (1995a) recommended the use of standard default diffusivity values. U.S. EPA (1995a) stated that the diffusivity parameters vary slightly, and default values appear to be within the range of typical values. Values for diffusivity in air range from about 0.01 to 0.1 square centimeters per second (cm^2/s); therefore, U.S. EPA (1995a) recommended a default value of 0.08 cm^2/s. Values for diffusivity in water range from 1×10^{-06} to 1×10^{-05} cm^2/s; therefore, U.S. EPA (1995a) recommended a default value of 8×10^{-06} cm^2/s. Diffusivity values calculated using Equations A-1-2a and A-1-2b were within the range specified by U.S. EPA (1995a).

PCDDs and PCDFs Diffusivity values in air and water for (1) 2,3,7,8-TCDD were obtained from U.S. EPA (1994c).

Metals and Mercuric compounds For metals (except chromium and mercury), diffusivity values were not available in the literature. Diffusivity values for chromium and mercury were obtained from the U.S. EPA (1994c) database. The diffusivity value for methyl mercury was calculated using Equations A-1-2a and A-1-2b.

Octanol/Water Partitioning Coefficient (K_{ow})

The *n*-octanol/water partitioning coefficient (K_{ow}) is defined as the ratio of the solute concentration in the water-saturated *n*-octanol phase to the solute concentration in the *n*-octanol-saturated water phase (Montgomery and Welkom 1991).

Organics KOWWIN version 1.67 was used to update DRAS K_{ow}s (U.S. EPA 2000). KOWWIN provides experimental references as well as a chemical structure-based model estimate of K_{ow}. Preference was given to reported experimental values, both within KOWWIN and the following references, over the use of modeled or estimated values.

K_{ow} values were also obtained from U.S. EPA (1994b). U.S. EPA (1994b) provides measured, calculated, and estimated K_{ow} values obtained from various literature sources. K_{ow} values that were not available in U.S. EPA (1994b) or KOWWIN were obtained from one of three sources, in the following order of preference:

1. U.S. EPA (1994e)

2. Karickhoff, S.W. and J.M. Long. 1995. "Internal Report on Summary of Measured, Calculated, and Recommended Log K_{ow} Values." Environmental Research Laboratory. Athens. April 10.

3. U.S. EPA (1995a), values from which were obtained from one of three sources:

    a. Mackay, D., W.Y. Shiu, and K.C. Ma. 1992. *Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Volume I - Monoaromatic Hydrocarbons, Chlorobenzenes, and PCBs. Volume II - Polynuclear Aromatic Hydrocarbons, Polychlorinated Dioxins and Dibenzofurans. Volume III - Volatile Organic Chemicals.* Lewis Publishers. Boca Raton, Florida.

    b. Howard, P.H. 1989-1993. *Handbook of Environmental Fate and Exposure Data For Organic Chemicals. Volumes I: Large Production and Priority Pollutants (1989). Volume II: Solvents (1990). Volume III: Pesticides (1991). Volume IV: Solvents2 (1993)*. Lewis Publishers. Chelsea, Michigan.

    c. Other literature sources, when values were not available in Mackay, Shiu, and Ma (1992) and Howard (1989-1993).

Metals No K_{ow} values were available for metals, either in the literature or in the primary guidance documents. K_{ow} values for the metals were assumed to be zero, because the affinity of the metals to the octanol is almost zero.

Mercuric compounds An experimental K_{ow} value for total mercury was obtained through KOWWIN. KOWWIN's estimated K_{ow} for methyl mercury was selected for DRAS. For mercuric chloride, the K_{ow} value was obtained from U.S. EPA (1997g).

Soil Organic Carbon-Water Partition Coefficient (K_{oc})

The soil organic carbon-water partition coefficient (K_{oc}) or the organic carbon normalized soil sorption coefficient is defined as the ratio of adsorbed compound per unit weight of organic carbon to the aqueous solute concentration (Montgomery and Welkom 1991).

Organics Because of the soil mechanisms that are inherently involved, K_{oc} values for the ionizing organics and nonionizing organics are discussed separately.

Ionizing Organic Compounds

Ionizing organic compounds include amines, carboxylic acids, and phenols. These compounds contain the functional groups that ionize under specific pH conditions, and include the following:

- Organic acids (2,4,6-trichlorophenol; pentachlorophenol; 2,3,4,5-tetrachlorophenol; 2,3,4,6-tetrachlorophenol; 2,4,5-trichlorophenol; 2,4-dichlorophenol; 2-chlorophenol; phenol; 2,4-dimethylphenol; 2-methylphenol; 2,4-dinitrophenol; and benzoic acid)

- Organic bases—n-nitroso-di-n-propylamine; n-nitrosodiphenylamine, and 4-chloroaniline)

K_{oc} values for ionizing organic compounds were obtained from U.S. EPA (1994b). U.S. EPA (1994b) provides K_{oc} values for the ionizing organic compounds that have been estimated on the basis of the degree of ionization and the relative proportions of neutral and ionized species. The primary guidance documents cite one value for the ionizing organics, independent of the pH. The primary guidance documents calculate K_{oc} values for the ionizing organics by using correlation equations containing K_{ow} that are applicable to nonionizing organics. However, K_{oc} values for ionizing compounds can vary vastly, depending on the pH conditions in the environment. For the ionizing organic compounds, the estimated K_{oc} values based on pH are provided.

K_{oc} values were estimated on the basis of the assumption that the sorption of ionizing organic compounds is similar to hydrophobic organic sorption, because the soil organic carbon is the dominant sorbent. According to U.S. EPA (1994b), for low pH conditions, these estimated values may over predict sorption coefficients, because they ignore sorption to components other than organic carbon.

Nonionizing Organic Compounds

Nonionizing organic compounds are all other organic compounds not listed earlier as ionizing. They include volatile organics, chlorinated pesticides, polynuclear aromatic hydrocarbons (PAHs), and phthalates. The geometric mean of measured K_{oc} values are provided in the following document:

- U.S. EPA. 1996a. *Soil Screening Guidance: Technical Background Document and User's Guide*. Office of Solid Waste and Emergency Response. Washington, DC. EPA/540/R-95/128. May.

U.S. EPA (1996a) calculated the geometric mean value from various measured values. For compounds for which K_{oc} values are not provided by U.S. EPA (1996a), K_{oc} values were calculated using K_{ow} correlation equations provided in the same document.

Metals For metals, no K_{oc} values were found in the literature. For metals, soil/sediment-water partitioning coefficients (*Kd*) were obtained directly from experimental measurements.

Chemical Partitioning, Partitioning Coefficients for Soil-Water (Kd_s) and Suspended Sediment-Surface Water (Kd_{sw})

Partition coefficients (*Kd*) describe the partitioning of a compound between sorbing material, such as soil, soil pore-water, surface water, suspended solids, and bed sediments. For organic compounds, *Kd* has been estimated to be a function of the organic-carbon partition coefficient and the fraction of organic carbon in the partitioning media. For metals, *Kd* is assumed to be independent of the organic carbon in the partitioning media and, therefore, partitioning is similar in all sorbing media.

The soil-water partition coefficient (Kd_s) describes the partitioning of a compound between soil pore-water and soil particles, and strongly influences the release and movement of a compound into the subsurface soils and underlying aquifer. The suspended sediment-surface water partition coefficient (Kd_{sw}) coefficient describes the partitioning of a compound between surface water and suspended solids or sediments.

Organics For organics (including PCDDs and PCDFs), soil organic carbon is assumed to be the dominant sorbing component in soils and sediments. Therefore, *Kd* values were calculated using the following fraction organic carbon (f_{OC}) correlation equations:

$$Kd_s = f_{oc,s} \cdot K_{oc} \qquad \text{Equation A-1-3a}$$

$$Kd_{sw} = f_{oc,sw} \cdot K_{oc} \qquad \text{Equation A-1-3b}$$

- U.S. EPA. 1993. *Review Draft Addendum to the Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions*. Office of Health and Environmental Assessment. Office of Research and Development. EPA-600-AP-93-003. November 10.

U.S. EPA (1993d), from literature searches, states that f_{OC} could range as follows:

- 0.002 to 0.024 in soils—for which a mid-range value of $f_{oc,s}$ = 0.01 generally can be used.
- 0.05 to 0.1 in suspended sediments—for which a mid-range value of $f_{oc,sw}$ = 0.075 generally can be used.

The DRAS uses mid-range f_{oc} values recommended by U.S. EPA (1993). *Kd* values were calculated using K_{oc} values recommended for each compound.

Metals For metals (except mercury), *Kd* is governed by factors other than organic carbon, such as pH, redox, iron content, cation exchange capacity, and ion-chemistry. Therefore, *Kd* values for metals cannot be calculated using the same correlation equations specified for organic compounds. Instead, *Kd* values for the metals must be obtained directly from literature sources. *Kd* values for all metals, except lead, were obtained from U.S. EPA (1996a). U.S. EPA (1996a) provides values for *Kd* that are based on pH, and are estimated by using the MINTEQ2 model, which is a geochemical speciation model. The MINTEQ2 model analyses were conducted under a variety of geochemical conditions and metal concentrations. The

MINTEQ2 pH-dependent *Kd* values were estimated by holding constant the iron oxide at a medium value and the f_{oc} at 0.002. For arsenic, hexavalent chromium, selenium, and thallium, empirical pH-dependent *Kd* values were used.

Kd value for lead was obtained from the following:

- Baes, C.F., R.D. Sharp, A.L. Sjoreen, and R.W. Shor. 1984. "Review and Analysis of Parameters and Assessing Transport of Environmentally Released Radionuclides Through Agriculture." Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Mercuric Compounds Both watershed erosion and direct atmospheric deposition can be important sources of mercury to a water body (U.S. EPA 1997g). There appears to be a great deal of variability in the processing of mercury among water bodies. This variability is primarily a result of the characteristically wide range of chemical and physical properties of water bodies that influence the levels of methylated mercury. Some of the mercury entering the water body is methylated predominately through biotic processes (U.S. EPA 1997g). In the absence of modeling site-specific water body properties and biotic conditions, consistent with U.S. EPA (1997g), U.S. EPA OSW recommends 85 percent of total mercury in surface water is assumed to be divalent mercury and the remaining mass as methyl mercury. For the fish ingestion pathway, the DRAS converts the total mercury in the surface water to the methyl mercury fraction by multiplying the total mercury concentration in a second order stream by 0.15 to determine the methyl mercury concentration. Kd_s values for mercury and methyl mercury were obtained from U.S. EPA (1996a). The *Kd* value for methyl mercury was obtained from U.S. EPA (1997g).

Aquatic Toxicity Reference Values (*Aquatic TRVs*)

Ecological benchmarks were developed for the protection of the aquatic community. These ecological benchmarks are referred to as toxicity reference values (TRVs) and were developed from a variety of ecological receptors based on the availability of data for a given waste constituent. The TRV is developed to protect the entire community, not one particular species. In general, TRVs (the measurement endpoints) were selected for consistency with the Agency's "Framework for Ecological Risk Assessment" (U.S. EPA 1992b). Region 6 believes the ecological analysis is conservative with respect to the overall assessment endpoint (e.g., sustainability of the reproducing populations) because of the way the source, fate and transport parameters are set and how the TRVs are developed.

The ecological assessment focused on inferring the sustainability of populations and communities within the aquatic ecosystem. Therefore, TRVs were derived from measurement endpoints (i.e., reproductive, developmental, growth, survival, and mortality) from which such inferences could be made. Reproductive studies (e.g., number of viable young per female) were preferred over other endpoints. The aquatic TRVs defaulted to a more conservative no effects level (or concentration) approach for ecological receptors. For populations of fish and aquatic invertebrates (represented by daphnids), a hierarchical approach was taken for use of data sources in deriving aquatic TRVs. The first choice was the final chronic values (FCVs) from the Ambient Water Quality Criteria (AWQC) effort by the EPA Office of Water (U.S. EPA 1998a). If these benchmarks were not available, then a freshwater aquatic TRV was selected from the draft *Protocol for Screening Level Ecological Risk Assessment at Hazardous Waste Combustion Facilities* (U.S. EPA. 1998b). Finally, TRVs were selected from the *Toxicological Benchmarks for Screening Potential contaminants of Concern for Effects on Aquatic Biota* (Suter and Tsao, 1996).

A.1.3 BIOTRANSFER FACTORS FOR ANIMALS

Bioconcentration and Bioaccumulation Factors for Chemicals in Fish

Bioconcentration and bioaccumulation factors for fish are used for various compounds, depending on the K_{ow} value of the organic compound. Bioconcentration factors for fish (BCF_{fish}) were used for organics with a log K_{ow} value less than 4.0; and for metals (except lead and mercury). Bioaccumulation factors for fish (BAF_{fish}) were used for organics with a log K_{ow} value greater than 4.0, lead, and mercuric compounds.

Bioconcentration Factors for Chemicals in Fish (BCF_{fish})

BCF_{fish} is the ratio of the chemical concentration in fish to the chemical concentration in the water column where the fish is exposed. It accounts for uptake of chemicals by fish from water passing across the gills. *BCF* values for fish were used for all organic compounds with a log K_{ow} of less than 4.0 (cutoff value with BAF_{fish}) and for all metals, except lead and mercury, as cited in U.S. EPA (1995a). This implies that the concentration of chemical in the fish is only due to water intake by the fish, and compounds with a log K_{ow} of less than 4.0 are assumed not to bioaccumulate.

BCF values reported in the DTSD Appendix are either:

1) Geometric mean of a valid number of field-measured values obtained from various field studies (or)
2) Geometric mean of laboratory-measured values obtained from various experimental studies (or)
3) Estimated values calculated using a correlation equation

NOTE: When only one valid field-measured value for a chemical was found in the literature, the higher of the field-measured value and the geometric mean of laboratory-measured values, was used.

In general, field measured BCFs were assumed to be based on total (dissolved and suspended) water column concentrations; and laboratory measured BCFs were assumed to be based on dissolved water column concentrations. This distinction is important for compounds with a log K_{ow} of greater than or equal to 4.0, because significant amounts of a chemical can partition into the suspended sediment organic carbon (or particulate phase) of the water column. For compounds with a log K_{ow} of less than 4.0, most of chemical is associated with the dissolved phase of the water column and negligible amounts of chemical is associated with the suspended sediment phase in the water column. Therefore, for compounds with a log K_{ow} of less than 4.0, BCF values based on dissolved chemical water concentrations in the water column are essentially the same as BCF values based on total (dissolved + suspended) chemical water concentrations in the water column.

The DTSD does not recognize differences in total versus dissolved water concentrations when calculating fish concentrations from BCF_{fish} values for compounds with a log K_{ow} of less than 4.0. Since, dissolved water concentrations is the major contributing factor from compounds with a log K_{ow} of less than 4.0, all BCF_{fish} values (irrespective of whether they were derived using total or dissolved water concentrations) can be multiplied by chemical concentration in the dissolved water column (C_{dw}) to calculate fish concentrations. This assumption is necessary because (1) literature data is often unclear if the water concentrations are dissolved or total concentrations, and (2) most of the literature reviewed indicated that

laboratory experiments were conducted using filtered or distilled water; or the experiments were conducted using fresh water, but were filtered before analyses for water concentrations.

Organics For organics with a log K_{ow} value of less than 4.0, BCF_{fish} values were obtained from either of two methods:

- Field-measured or laboratory-measured values from various experimental studies were evaluated by U.S. EPA (1998b). This information is summarized in the following document:

  U.S. EPA. 1998b. *Screening Level Ecological Risk Assessment Protocol for Hazardous Waste Combustion Facilities.* Draft Interim Final. April.

  Field-measured data is only (1) available for a limited number of compounds, and (2) based on a single study. In such cases, the field-measured value or the geometric mean of field-measured values were compared with the geometric mean of laboratory-measured values, and the higher one used. A detailed discussion on sources of BCF values and methodology followed are provided in Appendix C of U.S. EPA (1998b).

- When measured values were not available or could not be evaluated, the following correlation equation recommended by Lyman, Reehl, and Rosenblatt (1982) was used:

$$\log BCF_{fish} = -0.23 + 0.76 \log K_{ow} \qquad \text{Equation A-1-4}$$

Correlation Equation A-1-4 was developed by the following:

- Veith, G.D., K.J. Macek, S.R. Petrocelli, and J. Caroll. 1980. "An Evaluation of Using Partition Coefficients and Water Solubility to Estimate Bioconcentration Factors for Organic Chemicals in Fish." *Journal of Fish. Res. Board Can.* Prepublication Copy.

Veith, Macek, Petrocelli, and Caroll (1980) measured *BCF* values for four fish species in flow-through laboratory studies that were exposed to a wide range of organic chemicals. BCF_{fish} values calculated by using correlation Equation A-1-4 are (1) based on dissolved water concentrations, and (2) not lipid-normalized.

Metals For metals (except lead and mercury), BCF_{fish} values are measured values obtained from various literature studies, as cited in U.S. EPA (1998b). Measured values from various experimental studies were evaluated by U.S. EPA (1998b). Detailed discussion and sources of measured values were provided in U.S. EPA (1998b). For lead, a BAF is more applicable than a BCF as it tends to bioaccumulate.

Mercuric Compounds For mercuric compounds, a BAF is more applicable than a BCF as they tend to bioaccumulate. Therefore the BAF_{fish} value for methyl mercury was obtained from U.S. EPA (1997g) for a trophic level 4 fish.

Bioaccumulation Factors for Chemicals in Fish (BAF_{fish})

BAF_{fish} is the ratio of the chemical concentration in fish to the chemical concentration in the water body where the fish are exposed. The BAF_{fish} accounts for uptake of chemicals by fish from water and sediments passing across the gills, and from consumption of various foods including plankton, daphnids, and other

fish. BAFs for fish were used for organic compounds (except PCBs, PCDDs, and PCDFs) with a log K_{ow} greater than 4.0, lead and mercuric compounds.

For compounds with a log K_{ow} of greater than or equal to 4.0, chemicals can significantly partition into the suspended sediment organic carbon (or particulate phase) of the water column. Therefore, BAF values should be based on total (dissolved and suspended) water column concentrations. BAFs reported are either:

1) Geometric mean of field-measured values obtained from various experimental studies (or)
2) Predicted values calculated by multiplying a food chain multiplier (FCM) with a geometric mean of various laboratory measured BCFs. A FCM is the ratio of a BAF to a BCF, and is used to account for food chain biomagnification from a lower to a upper trophic level (or)
3) Predicted values calculated by multiplying a FCM with an estimated BCF. BCFs were estimated using correlation Equation A-1-4.

NOTE: When only one valid field-measured value for a chemical was found in the literature, the higher of the field-measured value and the geometric mean of laboratory-measured values, was used.

In general, (1) field-measured BAFs were assumed to be based on total (dissolved and suspended) water column concentrations, (2) laboratory-measured BCFs, and therefore, the BAFs predicted from them, were assumed to be based on dissolved water column concentrations, and (3) estimated BCFs using correlation Equation A-1-4, and therefore, the BAFs predicted from them, were assumed to be based on dissolved water column concentrations. In addition, field-measured BCFs, for compounds with a log K_{ow} greater than 4.0, were assumed to be equal to BAFs, because the tissue concentrations are a result of uptake of water (dissolved and suspended), sediment, and various trophic level food.

For consistency, all field-measured BAF (or BCF) values were adjusted according to the methodology specified in U.S. EPA (1995e) to include only the dissolved water column fractions; (i.e., the BAFs based on total water concentrations were converted to BAFs based on dissolved water concentrations). This was done, so that all BAF_{fish} values (based on dissolved water concentrations) can be multiplied by the chemical concentration in the dissolved water column (C_{dw}) to calculate fish concentrations.

In U.S. EPA (1995a), BAF values were estimated based on the models developed for the limnetic ecosystem by the following:

- Thomann, R.V. 1989. "Bioaccumulation Model of Organic Chemical Distribution in Aquatic Food Chains." *Environmental Science and Technology*. 23(6):699-707.

and, for the littoral ecosystem by the following:

- Thomann, R.V., J.P. Connolly, and T.F. Parkerton. 1992. "An Equilibrium Model of Organic Chemical Accumulation in Aquatic Food Webs with Sediment Interaction." *Environmental Toxicology and Chemistry*. 11:615-629.

BAF values were predicted by multiplying a laboratory-measured or predicted BCF by a FCM. The Thomann (1989) and Thomann, Connolly, and Parkerton (1992) models were adopted by U.S. EPA, Office of Water, for the Great Lakes Water Quality Initiative in 1993. In 1995, U.S. EPA, Office of Water, developed BAFs based on the following study:

- Gobas, F.A.P.C. 1993. "A Model for predicting the bioaccumulation of hydrophobic organic chemicals in aquatic food-webs: application to Lake Ontario." Ecological Modelling. 69:1-17.

The Gobas (1993) model was adopted to develop the latest water quality criteria and is provided in the following two documents:

- U.S. EPA. 1995d. *Water Quality Guidance for the Great Lakes System. Supplementary Information Document.* Office of Water. EPA-820-B-95-001. March.

- U.S. EPA. 1995e. *Great Lakes Water Quality Initiative. Technical Support Document for the Procedure to Determine Bioaccumulation Factors*. Office of Water. EPA-820-B-95-005. March.

The Gobas (1993) food-chain model was preferred because, unlike the Thomann (1989) model, it includes both benthic and pelagic food chains, thereby estimating exposure of organisms to compounds from both the sediment and the water column. Other inherent drawbacks of the Thomann (1989) model were that the model: (1) did not take into account metabolism, biotransformation, degradation, persistence, or seasonal or temporal variability, (2) is extremely sensitive to certain input parameter such as the lipid content, (3) incorrectly adopted FCMs, (4) is questionable in its assumption that the system is at steady state or in equilibrium, and (5) had little application for compounds with a log K_{ow} greater than 6.5, because the sediment route of exposure was not considered.

The Gobas (1993) model: (1) accounts for metabolism, but sets the metabolic rate to zero because of lack of data for individual compounds, (i.e., the metabolism is assumed not to occur), (2) incorporates the concentration of the compound in both the sediment and the water column, the sediment route being especially useful for compounds with a log K_{ow} greater than 6.5, and (3) includes the disequilibrium between concentrations of the compounds in sediment and the water column. Although the Thomann, Connolly, and Parkerton (1992) model accounts for sediment interaction, according to U.S. EPA (1995d), the Gobas (1993) model required fewer input parameters which could be more easily specified.

The following equation cited in U.S. EPA (1995e) was used to convert the BAF based on total water concentrations to a BAF based on dissolved water concentrations:

$$f_{fd} = \frac{1}{1 + \frac{(DOC)\ (K_{ow})}{10} + (POC)\ (K_{ow})} \qquad \text{Equation A-1-5}$$

where

f_{fd} = fraction of chemical that is freely dissolved in water
DOC = concentration of dissolved organic carbon, kg organic carbon / L water
POC = concentration of particulate organic carbon, kg organic carbon / L water

Since, the Gobas (1993) model was derived from a study conducted at Lake Ontario, DOC and POC values for Lake Ontario were used. Values cited in U.S. EPA (1995e) were:

$$DOC = 2 \times 10^{-6} \text{ kg/L}$$

POC = 7.5×10^{-9} kg/L

A BAF based on dissolved water concentrations can be calculated from a BAF based on total water concentrations as follows:

$$BAF\ (dissolved) = \frac{BAF\ (total)}{f_{fd}} - 1 \qquad \text{Equation A-1-6}$$

FCMs were obtained from Table 2 of U.S. EPA (1995e). U.S. EPA (1995e) provided FCMs as a function of log K_{ow} in increments of 0.1 for trophic level 2, 3, and 4 aquatic organisms. Humans are assumed to consume trophic level 3 or 4 fish. The higher FCM value of trophic levels 3 and 4 was used. When the log K_{ow} value of a chemical was between two log K_{ow} values listed in Table 2 of U.S. EPA (1995e), the FCM for the next highest log K_{ow} value was used.

Organics For all organics (except PCBs, PCDDs and PCDFs) with a log K_{ow} greater than or equal to 4.0, the FCM, which accounts for accumulation through the food chain in addition to water, becomes greater than 1. Therefore, a BAF_{fish}, which takes the food chain into consideration, is more appropriate than a BCF_{fish}.

For all organics with a log K_{ow} greater than or equal to 4.0, BAFs were derived using one of following three methods:

1) BAF = Field measured BAF or BCF, adjusted for dissolved water concentrations
2) BAF = Laboratory measured BCF multiplied by a FCM for either trophic level 3 or 4 fish
3) BAF = Estimated BCF calculated using correlation equation A-1-4 multiplied by a FCM for either trophic level 3 or 4 fish

Both field and laboratory measured values were derived from various literature sources cited in U.S. EPA (1998b). FCMs were obtained from U.S. EPA (1995e).

Metals (lead) For lead, the food-chain multiplier becomes greater than 1; therefore, a BAF is more appropriate. The BAF_{fish} value for lead was obtained as a geometric mean from various literature sources described in U.S. EPA (1998b). Since metals are assumed insoluble under neutral conditions, the dissolved and total water concentrations are almost equal. However, for consistency, the BAF_{fish} value for lead was adjusted for dissolved fractions.

Mercuric Compounds For mercuric compounds, a BAF is more applicable than a BCF as they tend to bioaccumulate. Therefore the BAF_{fish} value for methyl mercury was obtained from U.S. EPA (1997g) for a trophic level 4 fish.

A.1.4 HUMAN HEALTH BENCHMARKS

DRAS incorporates human health benchmarks as reference doses and reference concentrations for noncarcinogens, and as cancer slope factors for carcinogens. Reference dose (*RfD*) is defined as a daily intake rate of a compound estimated to pose no appreciable risk of deleterious effects over a specific exposure duration (U.S. EPA 1989). Reference concentration (*RfC*) is defined as the concentration of a compound estimated (with uncertainty spanning perhaps an order of magnitude) to pose no appreciable risk

of deleterious effects over a specific exposure duration (U.S. EPA 1989). EPA defines cancer slope factors as " used to estimate the risk of cancer associated with exposure to a carcinogenic or potentially carcinogenic substance. A slope factor is an upper bound, approximating a 95% confidence limit, on the increased cancer risk from a lifetime exposure to an agent by ingestion [or inhalation]".

Updated Toxicity Data

EPA reviewed all existing toxicity reference data in DRAS for outdated or errant values. To do so, EPA downloaded the 2004 version of the Region 9 Preliminary Remediation Goals (PRGs)(U.S. EPA 2004a) toxicity reference values to those in DRAS. We also reviewed Agency sources for any other changes which may have occurred after the 2004 PRG table was prepared.

Some of the updates were straightforward such as an unambiguous revision to the Integrated Risk Information System (IRIS – EPA's highest standard source for toxicity data). Other discrepancies required the review of Agency toxicologists in determining the appropriate default data for use in DRAS. In consideration of the exposure scenarios evaluated in the delisting program, EPA selected toxicity data in accordance with the hierarchy described in the December 2003 Memorandum from Michael B. Cook (U.S. EPA 2003), as did Region 9 in developing the 2004 PRG list. The types of pathway evaluations are very similar to those applied for Superfund-site evaluations. The hierarchy recommended is as follows:

> IRIS is the first tier of the recommended hierarchy as the generally preferred source of human health toxicity values. IRIS generally contains reference doses (RfDs),reference concentrations (RfCs), cancer slope factors, drinking water unit risk values, and inhalation unit risk values that have gone through a peer review and EPA consensus review process. IRIS normally represents the official Agency scientific position regarding the toxicity of the chemicals based on the data available at the time of the review.
>
> The second tier is EPA's [Provisional Peer Reviewed Toxicity Values] PPRTVs. Generally, PPRTVs are derived for one of two reasons. First, the [Superfund Health Risk Technical Support Center] STSC is conducting a batch wise review of the toxicity values in [the EPA Health Effects Summary Tables] HEAST (now a Tier 3 source). As such reviews are completed, those toxicity values will be removed from HEAST, and any new toxicity value developed in such a review will be a PPRTV and placed in the PPRTV database. Second, Regional Superfund Offices may request a PPRTV for contaminants lacking a relevant IRIS value. The STSC uses the same methodologies to derive PPRTVs for both.
>
> The third tier includes other sources of information. Priority should be given to sources that provide toxicity information based on similar methods and procedures as those used for Tier I and Tier II, contain values which are peer reviewed, are available to the public, and are transparent about the methods and processes used to develop the values. Consultation with the STSC or headquarters program office is recommended regarding the use of the Tier 3 values for Superfund response decisions when the contaminant appears to be a risk driver for the site. In general, draft toxicity assessments are not appropriate for use until they have been through peer review, the peer review comments have been addressed in a revised draft, and the revised draft is publicly available.

In October 2008, IRIS and PPRTV were checked once more for updates and added to DRAS in accordance with the Cook Memorandum.

Explanation of Calculated Toxicity Benchmark Values – Route-to-Route Extrapolation

To calculate missing benchmarks, available benchmarks can be employed using a methodology referred to as *route-to-route extrapolation*. Route-to-route extrapolation is when a toxicity factor for one route of exposure (i.e. ingestion) is converted into a toxicity factor for another route of exposure (i.e. inhalation). DRAS includes route-to-route extrapolations from the R9 2004 PRGs based on criteria set forth in "Methods for Derivation of Inhalation Reference Concentrations and Application of Inhalation Dosimetry" (U.S. EPA 1994g). Specifically, EPA believed that the most appropriate way to evaluate a large group of chemicals for route-to-route extrapolations was by applying the following criteria from the 1994 report:

> Oral data should not be used for route-to-route extrapolation in the following instances:
> (1) when groups of chemicals are expected to have different toxicity by the two routes; for example, metals, irritants, and sensitizers; . . .
> (6) when short-term inhalation studies, dermal irritation, in vitro-studies, or characteristics of the chemical indicate potential for portal-of-entry effects at the respiratory tract, but studies themselves are not adequate for an RfC development.

The following databases were used for the evaluation:

> (a) EPA's database for chemicals determined to be extremely hazardous substances after release to ambient air. These include chemicals assigned an EPA Level of Concern (LOC) as found in the document: "Technical Guidance for Hazards Analysis: Emergency Planning for Extremely Hazardous Substances" (U.S. EPA 1987);
>
> (b) Emergency Planning Response Guideline (ERPG) values for protection of the general public from the acute toxic and/or debilitating effects of chemicals in ambient air. ERPGs are developed by the American Industrial Hygiene Association (http://www.orau.gov/emi/scapa/erpgdefinitions.htm) (AIHA 2005);
>
> (c) U.S. DOE Temporary Emergency Exposure Limit (TEEL) values for protection of Federal workers and contractors at DOE facilities from the acute toxic and/or debilitating effects of chemicals in ambient air. TEELs are developed by methodologies similar to the ERPGs but include more chemicals (http://www.orau.gov/emi/scapa/teels.htm) (U.S. DOE 2005) ; and
>
> (d) NIOSH Recommended Exposure Limit (REL) values for work place exposure. This encompasses chemicals that have been assigned a specific time-concentration exposure limit in ambient air because they are documented to be respiratory irritants (even for a healthy worker) in ambient air in the absence of exposure protection. (www.cdc.gov/niosh/92-100.html) (U.S. DHHS 1992).

DRAS chemicals for which Region 9 recommends a route-to-route extrapolation also found in (a) include:

> Acrylamide; Aldrin; Benzyl Chloride; o-Cresol; Endosulfan; Endrin; Disulfoton; Furan; N-Nitrosodimethylamine; Parathion; Pentachlorophenol; Phenylmercuric acetate; Phorate;

DRAS chemicals for which Region 9 recommends a route-to-route extrapolation also found in (b) include:

Allyl chloride; Benzyl Chloride; Carbon tetrachloride; Methanol; Phenol; Trichloroethane (-1,1,1 and -1,1,2); Hexachlorobutadiene

DRAS chemicals for which Region 9 recommends a route-to-route extrapolation also found in (c) include:

Acrylamide; allyl chloride; aniline; benzo[a]pyrene; 2,4-dinitrophenol; dibenzo[a,h]anthracene; strychnine; hexachloroethane; hexachlorophene; chloromethane; tribromomethane; methanol; heptachlor; 1,2-dichloropropane; 1,1,2-trichloroethane; 1,1,2,2-tetrachloroethane; 1,1,1,2-tetrachloroethane; pentachloronitrobenzene; diethylphthalate; dibutylphthalate; pentachlorophenol; 2-chloronaphthalene; 3,3Æ-dichlorobenzidene; o-cresol; p-cresol; m-cresol; o-toluidene; 2-chlorophenol; 1,2,4,5-tetrachlorobenzene; 2,4,5-trichlorophenol; 1,3,5-trinitrobenzene; 1,3-dinitrobenzene; p-chloroaniline; pyridine; hexachlorobenzene; hexachlorobutadiene; 3,3-dimethoxybenzidine; 2,4-dichlorophenol; pentachlorobenzene; DDE;

DRAS chemicals for which Region 9 recommends a route-to-route extrapolation also found in (d) include:

Acetone - nose and throat irritant
Acetonitrile - nose and throat irritant
Bromoform - respiratory irritant
Dichlorobenzenes (all isomers) - upper respiratory irritants
Dichloroethylenes (all isomers) - mucous membrane irritants; narcosis;
Dimethylphthalate - upper respiratory irritant
Ethyl acetate - respiratory and eye irritant
Methyl acetate - upper respiratory irritant
Pentachlorophenol - upper respiratory irritant
Phenylenediamine - bronchial irritant and asthma inducer
Strychnine - convulsions
Trichloropropane - mucous membrane irritant; narcosis;

Consequently, for the above chemical constituents, we recommended against using route-to-route extrapolation from oral route data to derive inhalation toxicity factors.

For the remainder of the chemicals in the R9 2004 PRGs where extrapolation is used, the use of the route-to-route extrapolation in DRAS could be adopted on the basis that direct exposure effects of the remaining chemicals on the lung or respiratory system (of humans or animals) could not be identified. However, there could still be some significant uncertainties in the reliability of inhalation toxicity factors derived in this way. The primary uncertainty would probably be due to the rate of metabolism of a given chemical in the liver or lung and how that factor affects the ultimate level of absorption and transport to target organs. In the event that one of these route-to-route values becomes the basis for potentially denying a delisting petition, Region 5 recommends that the reference value be further investigated to reduce this uncertainty. In order to carry on the evaluation further, published literature studies on the metabolism or pharmacology of the individual chemicals would need to be located and reviewed.

The discussion above covers the concept of using route-to-route extrapolation from oral route data to derive inhalation toxicity factors. In the R9 2004 PRGs, there are also some instances where DRAS lists oral toxicity factors that were apparently derived from IRIS verified inhalation toxicity factors. The use of this extrapolation procedure would also be subject to uncertainty. For the purposes of making an expedited screening level evaluation, we propose the following caveat: the route-to-route extrapolation from

inhalation to oral should only be used when there is well documented evidence that exposure via the inhalation route results in adverse effects at organs or organ systems that are distant from the lung and respiratory tract (e.g., liver, kidney, thyroid, sex organs). The evaluation based on applying the above caveat is shown below:

RfD_O for Acetonitrile: IRIS reports health effects distant from the lung, therefore the route-to-route extrapolation is satisfactory.

RfD_O for Benzyl chloride: R9 lists an RfC referenced to NCEA. We recommend not using the route-to-route extrapolation until we are able to verify the health effects reported in this reference.

RfD_O for Chlorodifluoromethane: IRIS reports health effects distant from the lung, therefore the route-to-route extrapolation is satisfactory.

RfD_O for Chloromethane: Because IRIS states that exposure to chloromethane can essentially occur only through the vapor phase, derivation of an oral toxicity factor is not necessary.

RfD_O for 3-Chloropropene (Allyl chloride): IRIS reports peripheral neurological effects in humans and liver and kidney degenerative effects in lab animals; under the assumption that oral exposure to Allyl Chloride could occur, the route-to-route extrapolation is satisfactory;

RfD_O for 1,2-Dichloropropane: IRIS reports that the observed adverse effects were seen only in the nasal tissue and respiratory epithelium; therefore, route-to-route extrapolation should not be used;

RfD_O for 2-Nitropropane: IRIS reports development of focal hepatocellular nodules and focal liver necrosis in lab animals with no significant effects on the respiratory tract; under the assumption that oral exposure could occur to Nitropropane, the route-to-route extrapolation is satisfactory.

Provisional Toxicity Data, Multiple CAS ID Numbers, Multiple Valence States, and Data Based on a Mixture of Compounds

Approximately 26 potential waste constituents have provisional toxicity data, multiple CAS identification numbers, valence states, or toxicity data based on a mixture of compounds. We individually evaluated these using the following acronyms and conversion algorithms:

CSF_O – Oral Cancer Slope Factor
CSF_I – Inhalation Cancer Slope Factor
IUR – Inhalation Unit Risk (cancer)

RfD_O – Oral Reference Dose
RfD_I – Inhalation Reference Dose
RfC – Inhalation Reference Concentration

CalEPA – California EPA

Conversion of RfC to RfD_I:

$$RfD_I\ (mg/kg\text{-}day) = RfC\ (mg/m^3) \times (20\ m^3/day) \times (1/70\ kg) \qquad \text{Equation A1-7}$$

Conversion of IUR to CSF_I:

$$CSF_I = IUR(ug/m^3)^{-1} \times (1\ day/20\ m^3) \times (70\ kg) \times (1000\ ug/mg) \qquad \text{Equation A1-8}$$

Acrylonitrile

1) There is a single listed CAS number, therefore no problem.

2) The listed DRAS CSF_O is found in IRIS, therefore retain.

3) An IUR value of 6.8E-05 $(ug/m^3)^{-1}$ is found in IRIS and we used this value to calculate the CSF_I. The calculated CSF_I is 0.238 $(mg/kg\text{-}day)^{-1}$ which is the same as the listed DRAS value, therefore no change necessary.

4) An RfC value of 0.002 (mg/m^3) is found in IRIS, and we used this value to calculate RfD_I. The calculated RfD_I is 0.00057 (mg/kg-day); therefore we changed the listed DRAS value.

Arsenic

1) The listed DRAS values for CSF_O and RfD_O are correct values based on IRIS.

2) An IUR value of 4.3E-03 $(ug/m^3)^{-1}$ is found in IRIS, and we used this value to calculate a CSF_I of 15.05 $(mg/kg\text{-}day)^{-1}$. Since this is the same as the listed DRAS value, no change was necessary.

3) Note: IRIS has only one set of toxicity factors for Arsenic. These should be applied to analytical data for Ar(III), Ar (V) or Total Arsenic. For purposes of evaluating arsenic risk, EPA generally evaluates arsenic risk as Total arsenic unless a specific regulation spells out how arsenic should be analyzed and reported. If the DRAS program directs petitioners to report results for Ar(III) and Ar (V), there is still only one set of toxicity factors available.

4) We didn't need to use CalEPA values.

Benzo(k)fluoranthene

1) The listed DRAS CSF_O value of 0.073 $(mg/kg\text{-}day)^{-1}$ is correct based on use of the TEF factor approach based on the CSF_O for Benzo(a)pyrene.

2) The listed DRAS CSF_I of 0.031 $(mg/kg\text{-}day)^{-1}$ is the result of applying the TEF factor approach based on the EPA Region 4 finding of a published inhalation exposure study for Benzo(a)pyrene in hamsters as reported by NCEA (Thyssen 1981). This approach is more specific than just assuming route-to-route extrapolation from oral-to-inhalation exposure and therefore acceptable. This approach may be superseded when the Agency publishes a new IRIS file for PAHs.

Benzo(a)anthracene

The currently listed DRAS values are correct. The listed CSF_I of 0.31 $(mg/kg\text{-}day)^{-1}$ is acceptable based on the same rationale used above for Benzo(k)fluoranthene.

Benzo(b)fluoranthene

The currently listed DRAS values are correct. The listed CSF_I of 0.31 (mg/kg-day) $^{-1}$ is acceptable based on the same rationale used above for Benzo(k)fluoranthene.

Benzo(a)pyrene

The currently listed DRAS values are correct. The listed CSF_I of 3.1 (mg/kg-day) $^{-1}$ is acceptable based on the same rationale used above for Benzo(k)fluoranthene.

Chlordane

1) The listed DRAS CSF_O and CSF_I values are the same as IRIS values, therefore no change is necessary.

2) An RfC value of 0.0007 (mg/m^3)is found in IRIS and we used this value to calculate RfD_I of 0.0002 (mg/kg-day). We replaced the existing value with the new calculation.

3) IRIS states that the toxicology studies used to derive the toxicity factors were performed by administering Technical grade Chlordane to animals for both the oral and inhalation exposure routes. IRIS gives a definition of Technical grade Chlordane. Therefore, if the petitioner performs an analysis for Technical grade Chlordane or some other form of Chlordane, there is only one set of toxicity factors.

Chloroethane (Ethyl Chloride)

1) An RfC value of 10 (mg/m^3)is found in IRIS and we used this value to calculate RfD_I of 2.86 (mg/kg-day). We replaced the existing value with the new calculation.

2) The other listed DRAS toxicity values are correct.

3) The oral cancer slope factor could not be verified and a superseded document from NCEA did not match with R9's estimates of the inhalation slope factor, therefore we do not recommend that the carcinogenic toxicity factors be left blank at this time.

Chloroform

1) When the IRIS file for chloroform was revised (Oct. 2001), EPA made a significant change in its interpretation of the toxicological evidence. In particular, IRIS determined that ingested chloroform acts by non-linear Mode of Action – chloroform must induce cytotoxicity as a prerequisite for the induction of tumors in rodents. In addition, at dose levels below the oral RfD, chloroform does not induce the level of cytotoxicity and regenerative hyperplasia needed to induce the tumorigenic response. Therefore, the RfD was determined to be an adequate dose benchmark for cancer prevention. The following is the explanation found in the IRIS file:

> In the case of chloroform, the mode of action of carcinogenicity is reasonably well understood. Available data indicate that chloroform is not strongly mutagenic and chloroform is not expected to produce rodent tumors via a mutagenic mode of action (ILSI, 1997). Rather, there is good evidence that carcinogenic responses observed in animals are associated with regenerative hyperplasia that occurs in response to cytolethality (ILSI, 1997; U.S. EPA, 1998a,b). Because cytolethality occurs only at exposure levels above some critical dose level, a nonlinear approach is considered the most appropriate method for characterizing the cancer risk from chloroform.

> The Proposed Guidelines for Carcinogenic Risk Assessment (U.S. EPA, 1996) state that when the mode-of-action analysis based on available data indicates that the carcinogenic response is secondary to another toxicity that has a threshold, the margin-of-exposure analysis performed for toxicity is the same as is done for a noncancer endpoint, and an RfD for that toxicity may be considered in the cancer assessment. For chloroform, available evidence indicates that chloroform-induced carcinogenicity is secondary to cytotoxicity and regenerative hyperplasia; hence, the Agency relies on a nonlinear dose-response approach and the use of a margin-of-exposure analysis for cancer risk. The Agency has also chosen not to rely on a mathematical model to estimate a point of departure for cancer risk estimate, because the mode of action indicates that cytotoxicity is the critical effect and the reference dose value is considered protective for this effect.
>
> For more discussion of margin of exposure (MOE), see the Toxicological Review for Chloroform. Based on the kidney tumor of the drinking water study (Jorgenson et al., 1985), a point of departure (Pdp or LED10) of 23 mg/kg/day can be calculated using quantitative modeling of tumor dose-response data. Comparing the Pdp to the RfD of 0.01 mg/kg/day leads to a MOE of 2,000, which is considered large. Thus, in this case, the RfD for noncancer effect is also considered adequately protective of public health for cancer effects by the oral route, on the basis of the nonlinear dose response for chloroform and the mode of action for both cancer and noncancer effects having a common link through cytotoxicity.

We concluded that the existing CSF_O for chloroform be deleted and the Cal EPA cancer slope factor should not be adopted.

2) The listed DRAS CSF_I value should be rounded off to 0.081 $(mg/kg\text{-}day)^{-1}$.

3) The listed DRAS RfD_O value from IRIS is acceptable to use.

4) The 2004 Region 9 PRG referenced a value from NCEA for the RfC, 0.049 mg/m^3. We could not locate this reference. The latest Region 9 PRG (2008) lists a value derived from ATSDR. An RfC of 9.93E-02 (mg/kg day) was derived from a chronic inhalation minimum risk level (MRL) published by ATSDR in 1997.

Chromium

1) For Cr(III), IRIS states that the following factors cannot be developed: RfC (RfD_I), CSF_O, and IUR (CSF_I); therefore deleted those values from DRAS; for Cr(III), DRAS lists only an RfD_O of 1.5 (mg/kg-day).

2) For Cr (VI), the listed DRAS RfD_O is correct;

3) Since the IRIS RfC is 8E-06 (mg/m^3) the DRAS RfD_I should be 2.3E-06 (mg/kg-day). This RfD_I is for Cr(VI) mists and aerosols (e.g., chromium plating operations). If the potential exposure is more likely to be from Cr(VI) particulates, IRIS suggests that an RfC of 1E-04 (mg/m^3) should be used, and the corresponding RfD_I is 2.9E-05 (mg/kg-day).

4) For Cr (VI), the IRIS IUR is 1.2E-02 $(ug/m^3)^{-1}$ and the calculated CSF_I is 42 $(mg/kg\text{-}day)^{-1}$. As stated in IRIS, industrial worker exposure was known to be from Cr(VI)-Cr(III) mixtures, so there is some

uncertainty in the actual slope factor that would be due to Cr(VI) alone. The Cr(VI):Cr(III) ratio was assumed to be at least 1:6 for development of the slope factor; therefore, the highest possible CSF_I would be 7 x 42 = 294 $(mg/kg\text{-}day)^{-1}$. Therefore, we used this latter value if exposure needs to be modeled as due to Cr(VI) alone; if the suspected exposure would be due to a mixture of valences, we suggest using the 42 $(mg/kg\text{-}day)^{-1}$ value.

Chrysene

The currently listed DRAS values are correct. The listed CSF_I of 0.0031 $(mg/kg\text{-}day)^{-1}$ is acceptable based on the same rationale used above for Benzo(k)fluoranthene.

Cumene

1) The listed DRAS RfD_O is correct.

2) Since the IRIS RfC is 0.385 (mg/m^3), the calculated RfD_I should be 0.11 (mg/kg-day).

Dibenz(a,h)anthracene

The currently listed DRAS values are correct. The listed CSF_I of 3.1 $(mg/kg\text{-}day)^{-1}$ is acceptable based on the same rationale used above for Benzo(k)fluoranthene.

1,2-Dibromo-3-chloropropane

1) Since the IRIS RfC value is 0.0002 (mg/m^3), the calculated DRAS RfD_I should be 5.71E-05 (mg/kg-day);

2) The EPA Region 9 PRG reference from 2004 originally recommended a route-to-route extrapolation for RfD. However, EPA Superfund has since provided a provisional RfD_O under PPRTV and that value is used as the default in DRAS.

3) The EPA Region 9 PRG reference from 2004 originally recommended slope factors from California EPA. However, EPA Superfund has since provided provisional slope factors under PPRTV and those values are used as the default in DRAS.

1,1-Dichloroethane

1) The listed HEAST RfC value of 0.5 (mg/m^3) is correct and is the only provisional toxicity factor available until the IRIS file is revised. Therefore, the calculated RfD_I value should be 0.143 (mg/kg-day) in DRAS;

2) The EPA Region 9 PRG reference from 2004 originally recommended a route-to-route extrapolation for RfD. However, EPA Superfund has since provided a provisional RfD_O under PPRTV and that value is used as the default in DRAS.

3) There are no acceptable cancer slope factors available for this chemical. We suggest not using the CalEPA listed slope factors that were derived from an NCI 1977 study in rats. The EPA IRIS program re-evaluated this study and determined that it contained too many confounding results to use for deriving a CSF_O value.

Dichloropropane (cis-, trans-, mixture)

1) In the "mixture" heading, all of the listed DRAS values are correct except for the RfD_I. Since the IRIS RfC value is 0.02 (mg/m^3), the calculated DRAS RfD_I should be 0.00571 (mg/kg-day);

2) For the cis- and trans- isomers, DRAS has an additional value of 0.175 $(mg/kg\text{-}day)^{-1}$ for the CSF_O. We could not determine where it came from and do not think it should be used;

Dinitrotoluene (2,4-; 2,6-; mixture)

2,4-DNT: The current DRAS RfD_O is correct. It should be acceptable to use the CSF_O listed for the "mixture" since it is found on IRIS. We could not determine the origin of the values listed for RfD_I and RfC, so we suggest not using.

2,6-DNT: The CSF_O value listed for the mixture is the only available toxicity factor that we believe is appropriate. However, EPA Superfund has since provided a provisional RfD_O under PPRTV for this isomer and that value is used as the default in DRAS. We could not determine the origin of the values listed for RfD_I and RfC, so suggest not using;

Mixture-DNT: The CSF_O value listed for the mixture is the only available toxicity factor that we think is appropriate to use.

Epichlorohydrin

1) The current listed DRAS CSF_O value of 0.0099 $(mg/kg\text{-}day)^{-1}$ is correct.

2) Since the listed IRIS IUR value is 1.2E-06 $(ug/m^3)^{-1}$, the calculated DRAS CSF_I should be 0.0042 $(mg/kg\text{-}day)^{-1}$ (and the reference to HEAST can be changed to IRIS).

3) Since the IRIS RfC is 0.001 (mg/m^3), the calculated DRAS RfD_I should be 0.00029 (mg/kg-day).

4) Although IRIS has withdrawn the original RfD_O value. EPA Superfund has provided a provisional RfD_O under PPRTV and that value is used as the default in DRAS.

HCH and Lindane

1) The currently listed DRAS values appear to be correct.

2) For the missing DRAS RfD_O value under "beta-" and "alpha-", EPA Region 9 PRGs recommended using the NCEA provisional values shown under the PRG column. However, this reference could not be located. The latest Region 9 PRG (2008) lists values derived from ATSDR. RfD_Os of 8.0E-03 mg/kg day and 6.0E-04 mg/kg day were derived from inhalation minimum risk levels (MRLs) for alpha-HCH and beta-HCH, respectively, published by ATSDR in 2005.

3) For "gamma-" use a CSF_I value of 1.3 $(mg/kg\text{-}day)^{-1}$ because IRIS used a route-to-route extrapolation for "alpha"- and "beta-" to derive a CSF_I from the CSF_O.

4) For the RfD_I, we assume that route-to-route extrapolation from oral exposure is valid, and use the values listed in the PRG column as the values to adopt for DRAS.

Hexahydro-trinitro-triazene (RDX)

1) The listed DRAS values for CSF_O and RfD_O are correct.

2) We recommend using the CSF_I value and RfD_I value obtained from route-to-route extrapolation. The reason is that we were not able to find information showing that RDX is a sensitizer, irritant, or is acutely toxic by the inhalation route.

Indeno(1,2,3-cd)pyrene

The currently listed DRAS values are correct. The listed CSF_I of 0.31 $(mg/kg\text{-}day)^{-1}$ is acceptable based on the same rationale used above for Benzo(k)fluoranthene.

Lead

There are no IRIS cancer slope factors or Reference Doses for lead. EPA bases the protective media concentration on an uptake-absorption model in children up to seven years old in the child model; and for a pregnant woman in the adult model (to provide protection to the adult and the unborn child).

The general cleanup program policies are: lead releases to residential soil should not cause total soil lead concentration to exceed 400 (mg/kg); lead releases to industrial/commercial use soil (i.e., adult only exposure) should not cause total soil concentration to exceed 800 (mg/kg);

Mercury

1) The CASRN of 7439-97-6 means Hg(0) or elemental mercury. The listed DRAS RfD_I value and RfC value are correct however, there is no RfD_O value for Hg(0), so it is not appropriate to use the value from methyl mercury.

2) Mercury and compounds: This for the inorganic Hg valence states above zero, including Hg(II), such as HgCl2 and HgO. The only available toxicity factor is the RfD_O of 0.0003 (mg/kg-day).

3) Methyl mercury: This is for organic mercury that has accumulated and bioconcentrated in organic tissues (e.g., fish, wildlife). The only available toxicity factor is the RfD_O of 0.0001 (mg/kg-day). This constituent is not easy to measure accurately in tissues. So the default assumption is that all mercury detectable in organic tissues is methyl mercury;

4) DRAS currently includes separate constituents of concern for mercury and methyl mercury due to the differences in both toxicity and fate and transport in the environment. Methyl mercury is listed as *Mercury (Fish Pathway Only)* while all other forms of mercury are evaluated under *Mercury.*

Naphthalene

1) The listed DRAS RfD_O is correct. Since the IRIS RfC is 0.003 (mg/m^3), the DRAS RfD_I should be 8.6E-04 (mg/kg-day).

2) We recommend in this case that DRAS include the provisional Cancer Slope Factor for Naphthalene, even though the final decision has not yet been published in IRIS. The peer review draft of the Toxicological Review document (2004) states EPA's finding that Naphthalene should be regarded as a probable human carcinogen by the inhalation route. The proposed IUR is 1E-04 $(ug/m^3)^{-1}$. The calculated provisional CSF_I is 0.35 $(mg/kg\text{-}day)^{-1}$.

3) It would not be appropriate to use route-to-route extrapolation to derive a CSF_O from the provisional CSF_I. The Toxicological Review document mentioned above specifically states that the data on oral exposure were inadequate to support derivation of a CSF_O.

Nickel

1) The CASRN of 7440-02-0 is for nickel salts or nickel compounds. The listed DRAS RfD_O of 0.02 (mg/kg-day) should be used for ingestion of all forms of nickel except nickel subsulfide as explained below.

2) Use the listed R9 CSF_I of 0.84 $(mg/kg\text{-}day)^{-1}$ for inhalation of all forms of nickel except nickel subsulfide as explained below. We did not assume route-to-route extrapolation to derive a CSF_O value.

3) If nickel subsulfide needs to be retained as a DRAS constituent because of a specific industrial process, we can use the listed R9 CSF_I value of 1.7 $(mg/kg\text{-}day)^{-1}$ as the DRAS value for CSF_I. We did not assume route-to-route extrapolation to derive a CSF_O value.

Polychlorinated biphenyls (PCBs) (Aroclors)

In most PCB analyses performed by the historical EPA method, the results are presented as an amount of total Aroclors and/or amounts of specific Aroclors (1254, 1260, 1248, etc.). This gives very little information about the actual level of chlorination in the mixture. So when Aroclor analysis is performed, assume that the mixture is highly chlorinated and use the "high risk" slope factors: $CSF_O = 2$ $(mg/kg\text{-}day)^{-1}$; and $CSF_I = 2$ $(mg/kg\text{-}day)^{-1}$.

For non-cancer hazard, assume that the mixture is composed of the most hazardous Aroclor (1254) and use the $RfD_O = 0.00002$ (mg/kg-day). In this case, it is acceptable to use route-to-route extrapolation and apply an RfD_I value of 0.00002 (mg/kg-day) because of evidence that inhalation exposure of PCBs can result in adverse effects at distant sites from the lung.

To apply the "low risk" toxicity factors, the petitioner needs to perform a more refined sample analysis. For example, to obtain evidence for a low risk mixture, GC-MS analysis needs to be performed to accomplish an isomer group analysis that will report the results as mono- through deca- PCB homologs. This will yield more specific data about the chlorine content of the mixture. Then IRIS states that the mixture should be assumed to be low risk only if "congener or isomer analyses verify that congeners with more than 4 chlorines comprise < 0.5% of the total PCBs." And by analogy, only apply the highest RfD_O of 0.00007 (mg/kg-day) if analysis shows that the chlorine content is very low or if the mixture can be verified to be composed of only Aroclor 1016.

TCDD, 2,3,7,8

The listed DRAS CSF_O and CSF_I are correct. The only available source of toxicity factors is HEAST until the EPA finalizes the Dioxin Reassessment.

Tetrachloroethylene (PCE)

The CalEPA values are acceptable as the most recent data from an approved tertiary source of reference data according to the Cook memo.

The CalEPA provisional toxicity factors are: CSF_O = 0.54 (mg/kg-day) $^{-1}$;
CSF_I = 0.021 (mg/kg-day) $^{-1}$ (based on an IUR of 5.9E-06 (ug/m^3) $^{-1}$; and
Chronic Inhalation REL = 35 (mg/m^3).
Thus, the RfC = 0.035 (mg/m^3), RfD_I is 0.035 times 20 (m^3/day) divided by 70 kg = 0.01 (mg/kg-day).

The listed IRIS RfD_O is 0.01 (mg/kg-day). In this case, it is acceptable to apply route-to-route extrapolation since studies of inhalation exposure in mice showed that exposure by this route resulted in liver toxicity and liver tumors. Then the RfD_I is 0.01 (mg/kg-day).

Trichloroethylene (TCE)

There is a recent EPA risk assessment which received external peer review (Trichloroethylene Health Risk Assessment: Synthesis and Characterization; ORD 2001). This document recommended some toxicity factors, in particular, a new cancer slope factor. However, EPA decided not to move ahead and finalize the RA document or the new IRIS file because of internal and external disagreement over some of the data analysis in the RA document. EPA has since initiated a consultation with the National Academy of Science to review parts of the RA document. When the review is complete, EPA will finalize the RA document and the IRIS file. But this will take some time. Meanwhile, NCEA has been reluctant to support the proposed new cancer slope factor or recommend using it as the provisional value. Therefore, as with PCE, the CalEPA values are acceptable as the most recent data from an approved tertiary source of reference data according to the Cook memo.

The CalEPA provisional toxicity values are: CSF_O = 0.013 (mg/kg-day) $^{-1}$; CSF_I = 0.007 (mg/kg-day) $^{-1}$;
Chronic Inhalation REL = 600 (mg/m^3) thus, RfC = 0.600 (mg/m^3), RfD_I is 0.600 times 20 (m^3/day) divided by 70 kg = 0.17 (mg/kg-day).

The only existing RfD_O is 0.006 (mg/kg-day) originally provided by NCEA. The 2001 document with the new CSF also includes a new RfD_O which is also under review. The DRAS will use the provisional external review draft RfD_O of 3.0E-04 (mg/kg day) as the default value.

Trichlorophenol 2,4,6-

1) DRAS should use the listed IRIS values for CSF_O, 0.011 (mg/kg-day)$^{-1}$, and CSF_I, 0.011 (mg/kg-day)$^{-1}$.

2) DRAS should use the NCEA provisional value for RfD_O. Also, we used route-to-route extrapolation of the NCEA RfD_O to obtain the RfD_I because IRIS used route-to-route extrapolation to obtain the IUR from the CSF_O.

Vinyl Chloride

DRAS should use all the listed IRIS toxicity factors which are: CSF_O = 1.4 (mg/kg-day) $^{-1}$; CSF_I = 0.031 (mg/kg-day) $^{-1}$ [based on IUR = 8.8E-06 (ug/m^3) $^{-1}$]; RfD_O = 0.003 mg/kg-day; and RfD_I = 0.0286 mg/kg-day [based on RfC = 0.1 mg/m^3].

DRAS Constituents Not in R9 PRG Table

Acetaldehyde

1) The listed IRIS RfC is 0.009 (mg/m^3). Therefore, the RfD_I should be 0.0026 (mg/kg-day).

2) The listed IRIS IUR is 2.2E-06 (ug/m^3) $^{-1}$. Therefore, the CSF_I should be 0.0077 (mg/kg-day) $^{-1}$.

3) We do not use route-to-route extrapolation to derive a DRAS CSF_O because this chemical could have direct acute exposure effects in the lung or respiratory system.

Acetophenone

The listed IRIS RfD_O is 0.1 (mg/kg-day).

Bis(2-chloroisopropyl)ether

The listed IRIS RfD_O is 0.04 (mg/kg-day).

We could not determine the origin of the listed DRAS cancer slope factors.

Bromophenyl phenylether

We could not verify any useable toxicity factors including from HEAST or CalEPA. The original source listed in DRAS as a reference, the 1997 Region 3 RBCs, no longer lists this COC. This constituent should become "factorless."

Chloromethane

IRIS gives an RfC from which an RfD_I can also be calculated. No cancer data was given and oral pathways were specifically discouraged by IRIS because chloromethane is primarily a gas.

Chlorophenyl phenylether

We could not verify any useable toxicity factors including from HEAST or CalEPA. We think that this constituent should become "factorless."

Dichloroethylene - 1,1

1) IRIS withdrew the CSF_O and the IUR because a formal review concluded that the existing data do not support the development of cancer slope factors. This constituent should be treated as a non-carcinogen.

2) The RfD_O should be 0.05 (mg/kg-day).

3) Since the IRIS RfC is 0.2 (mg/m^3), the DRAS RfD_I should be 0.057 (mg/kg-day).

Dimethylbenz[a,h]anthracene

Because CalEPA has developed an oral cancer slope, the CalEPA value can be used in place of the HEAST value.

The CalEPA CSF_O is 250 $(mg/kg\text{-}day)^{-1}$.

Ethyl methanesulfonate

It would be acceptable to use the listed HEAST value. However, we could not find this value in the 1997 HEAST table.

3-Methylcholanthrene

Because CalEPA has developed an oral cancer slope, the CalEPA value can be used in place of the HEAST value.

The CalEPA CSF_O is 22 $(mg/kg\text{-}day)^{-1}$.

4-Nitrophenol

We could not verify any useable toxicity factors including from HEAST or CalEPA. The original source listed in DRAS as a reference, the 1997 Region 3 RBCs, no longer lists this COC. This constituent should become "factorless."

N-Nitrosopiperidine

We could not verify any toxicity factors in IRIS or HEAST.

Because CalEPA has developed an oral cancer slope, the CalEPA value can be used.

The CalEPA CSF_O is 9.4 $(mg/kg\text{-}day)^{-1}$.

Tris(dibromopropyl)phosphate

We could not verify any toxicity factors in IRIS or HEAST.

Because CalEPA has developed an oral cancer slope, the CalEPA value can be used.

The CalEPA CSF_O is 2.3 $(mg/kg\text{-}day)^{-1}$.

New Toxicity Data - Subsequent to the R9 PRG 2004 Review

IRIS and PPRTV were checked to ensure that any changes or updates subsequent to the 2004 R9 PRG review are included in DRAS. The following updates were included:

Ethylene Dibromide CASRN 106-93-4

The toxicity factors currently available in IRIS are:

CSF_O = 2 (mg/kg-day) $^{-1}$
IUR = 0.006 (ug/m^3) $^{-1}$
Therefore, the DRAS CSF_I should be 2.1 (mg/kg-day) $^{-1}$.

RfD_O = 0.009 (mg/kg-day)
RfC = 0.009 (mg/m^3)
Therefore, the DRAS RfD_I should be 0.0026 (mg/kg-day).

Toluene CASRN 108-88-3

The revised toxicity factors currently available in IRIS are:

RfD_O = 0.08 (mg/kg-day)
RfC = 5 (mg/m^3)
Therefore, the DRAS RfD_I should be 1.4286 (mg/kg-day).

Barium CASRN 7440-39-3

The revised toxicity factor currently available in IRIS is:

RfD_O = 0.2 (mg/kg-day).

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TABLE A-1-1

CHEMICAL-SPECIFIC INPUTS FOR ACENAPHTHENE (83-32-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	154.21
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	368.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.93E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.80E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.00E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.21E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.19E-06
Log K_{ow} (unitless)	Hansch (1995)	3.92
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.90E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.90E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.67E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.3E-01
$\hat{o}$ (hr)	ô value was obtained from U.S. EPA (1992b).	7.60E-01
*t** (hr/event)	t* value was obtained from U.S. EPA (1992b).	6.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	8.30E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	5.61E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-1

CHEMICAL-SPECIFIC INPUTS FOR ACENAPHTHENE (83-32-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	6.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	2.10E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	17

Note: NA = Not applicable, ND = No data available

TABLE A-1-2

CHEMICAL-SPECIFIC INPUTS FOR ACENAPTHYLENE (208-96-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	152.20
T_m (K)	CRC Handbook (1995)	365.65
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was cited from CRC Handbook (1995).	8.29E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.39E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.53E-06
Log K_{ow} (unitless)	Hansch (1995)	3.94
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.55E-01
t	ô value was obtained from U.S. EPA (1992b).	7.42E-01
*t** (hr/event)	t* value was obtained from U.S. EPA (1992b).	6.23E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.00E+00
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-2

CHEMICAL-SPECIFIC INPUTS FOR ACENAPTHYLENE (208-96-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	NA
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	NA
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-3

CHEMICAL-SPECIFIC INPUTS FOR ACETALDEHYDE (75-01-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	154.21
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	368.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.93E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.80E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.00E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.21E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.19E-06
Log K_{ow} (unitless)	TSCATS	-0.34
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.90E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.90E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.67E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.3E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	7.60E-01
*t** (hr/event)	t* value was obtained from U.S. EPA (1992b).	6.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	8.30E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.24E+-1
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-3

CHEMICAL-SPECIFIC INPUTS FOR ACETALDEHYDE (75-01-0)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	9.00E-03
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	7.70E-03
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	17

Note: NA = Not applicable, ND = No data available

TABLE A-1-4

CHEMICAL-SPECIFIC INPUTS FOR ACETONE (67-64-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	58.08
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	179.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.99E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	6.04E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.88E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.87E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.15E-05
Log K_{ow} (unitless)	Hansch (1995).	-0.24
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.81E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.81E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.36E-02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.70E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.00E-01
*t** (hr/event)	t* value was obtained from U.S. EPA (1992b).	4.70E-01
B	*B* value was obtained from U.S. EPA (1992b).	5.80E-05

TABLE A-1-4

CHEMICAL-SPECIFIC INPUTS FOR ACETONE (67-64-1)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)	4.00E-01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	9.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Suter (1996)	1.5E+03

Note: NA = Not applicable, ND = No data available

TABLE A-1-5

CHEMICAL-SPECIFIC INPUTS FOR ACETONITRILE (75-05-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	41.05
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	318.1
Vp (atm)	Howard (1989-1993)	1.20E-01 at 25°C (solid)
S (mg/L)	Howard (1989-1993)	1.30E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.79E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.14E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.40E-05
Log K_{ow} (unitless)	Hansch (1995).	-0.34
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.44E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.64E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.38E-02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	6.10E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.60E-01
*t** (hr/event)	t* value was obtained from U.S. EPA (1992b).	3.70E-01
B	*B* value was obtained from U.S. EPA (1992b).	4.60E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.25E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-5

CHEMICAL-SPECIFIC INPUTS FOR ACETONITRILE (75-05-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	Route to route extrapolation from RfC.	1.70E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	6.0E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-6

CHEMICAL-SPECIFIC INPUTS FOR ACETOPHENONE (98-86-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	120.50
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	293.6
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	5.20E-04 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	6.10E+03
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.03E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.73E-06
Log K_{ow} (unitless)	Hansch (1995).	1.58
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.58E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.58E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.68E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.10E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.70E-01
*t** (hr/event)	t* value was obtained from U.S. EPA (1992b).	1.10E+00
B	*B* value was obtained from U.S. EPA (1992b).	4.40E-03

TABLE A-1-6

CHEMICAL-SPECIFIC INPUTS FOR ACETOPHENONE (98-86-2)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	9.35E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-7

CHEMICAL-SPECIFIC INPUTS FOR ACROLEIN (107-02-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	56.06
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	185.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	3.50E-01 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	2.10E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.34E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.92E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.22E-05
Log K_{ow} (unitless)	Hansch (1995).	-0.01
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.18E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.18E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.82E-02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	8.50E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.90E-01
*t** (hr/event)	t* value was obtained from U.S. EPA (1992b).	4.60E-01
B	*B* value was obtained from U.S. EPA (1992b).	9.80E-05

TABLE A-1-7

CHEMICAL-SPECIFIC INPUTS FOR ACROLEIN (107-02-8)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	5.79E-01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	2.0E-05
Inhalation URF $(\mu g/m^3)^{-1}$	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	2.1E+00

Note: NA = Not applicable, ND = No data available

TABLE A-1-8

CHEMICAL-SPECIFIC INPUTS FOR ACRYLAMIDE (79-06-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	71.08
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	357.65
Vp (atm)	*Vp* value cited in U.S. EPA (1995g)	9.20E-06
S (g/100ml H_2O)	Geometric mean value cited in U.S. EPA (1994c).	2.15E+02
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g)	3.00E-10
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.70E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.06E-05
Log K_{ow} (unitless)	Hansch (1995).	-0.67
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.53E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.53E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.65E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.50E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.40E-01
*t** (hr/event)	t* value was obtained from U.S. EPA (1992b).	5.70E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.10E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.82E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-8

CHEMICAL-SPECIFIC INPUTS FOR ACRYLAMIDE (79-06-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.00E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	4.50E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	4.55E+00
MCL	National Primary Drinking Water Regulations.	1.00E+00 TT
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-9

CHEMICAL-SPECIFIC INPUTS FOR ACRYLONITRILE (107-13-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	53.06
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	189.6
Vp (atm)	*Vp* value cited in U.S. EPA (1995g) .	1.40E-01 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g) .	7.50E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.90E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.11E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.23E-05
Log K_{ow} (unitless)	Hansch (1995).	0.25
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.89E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.89E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.42E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.43E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.80E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.40E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.80E-04

TABLE A-1-9

CHEMICAL-SPECIFIC INPUTS FOR ACRYLONITRILE (107-13-1)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)	4.80E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	1.0E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	5.4E-01
RfC (mg/m^3)	U.S. EPA (2004b)	2.0E-03
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	2.4E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	7.6E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-10

CHEMICAL-SPECIFIC INPUTS FOR ALDRIN (309-00-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	364.93
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	377.1
Vp (atm)	*Vp* value cited in U.S. EPA (1994b).	2.20E-08 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1994b).	7.84E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.35E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.43E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.40E-06
Log K_{ow} (unitless)	DeBruijn (1989).	6.5
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.87E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.87E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.65E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	4.70E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.50E+01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	6.90E+01
B	*B* value was obtained from U.S. EPA (1992b).	3.20E+02

TABLE A-1-10

CHEMICAL-SPECIFIC INPUTS FOR ALDRIN (309-00-2)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAF*s were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	1.32E+06
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.00E-05
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.70E+01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.70E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	3E-01

Note: NA = Not applicable, ND = No data available

TABLE A-1-11

CHEMICAL-SPECIFIC INPUTS FOR ALLYL CHLORIDE (107-05-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	76.53
T_m (K)	Montgomery and Welkom (1991)	138.65
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	4.80E-01
S (mg/L)	*S* value cited in U.S. EPA (1995g).	3.40E+03
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g)	1.10E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.17E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.08E-05
Log K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	1.45
K_{oc} (mL/g)	K_{cw} value cited in U.S. EPA (1995g).	2.70E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.70E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.02E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	7.00E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.60E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	6.20E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.80E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	7.44E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-11

CHEMICAL-SPECIFIC INPUTS FOR ALLYL CHLORIDE (107-05-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	Route to route extrapolation from RfC.	2.90E-04
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	1.00E-03
Inhalation [1] *CSF* (mg/kg/day)$^{-}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-12

CHEMICAL-SPECIFIC INPUTS FOR ANILINE (62-53-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	93.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	266.8
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	8.80E-04 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	3.60E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	2.28E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.56E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.01E-05
Log K_{ow} (unitless)	Hansch (1995).	0.9
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.67E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.67E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.75E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.60E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.20E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.80E-01
B	*B* value was obtained from U.S. EPA (1992b).	9.50E-04

TABLE A-1-12

CHEMICAL-SPECIFIC INPUTS FOR ANILINE (62-53-3)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.84E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004c)	7.0E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	5.7E-03
RfC (mg/m^3)	U.S. EPA (2004b)	1.00E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-13

CHEMICAL-SPECIFIC INPUTS FOR ANTHRACENE (120-12-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	178.22
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	491.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	3.35E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	5.37E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.11E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.24E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.74E-06
Log K_{ow} (unitless)	Hansch (1995).	4.45
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.35E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.35E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.76E+03
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	2.61E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.07E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.50E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.47E+00

TABLE A-1-13

CHEMICAL-SPECIFIC INPUTS FOR ANTHRACENE (120-12-7)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	2.51E+03
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.1E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Suter (1996)	7.3E-01

Note: NA = Not applicable, ND = No data available

TABLE A-1-14

CHEMICAL-SPECIFIC INPUTS FOR ANTIMONY (7440-36-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	121.75
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	903.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	NA
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.73E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.96E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	45 at pH=6.8
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e).	45 at pH=6.8
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	--	ND
ô (hr/event)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b)	4.00E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-14

CHEMICAL-SPECIFIC INPUTS FOR ANTIMONY (7440-36-0)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1998b)	4.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	6E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.60E+2

Note: NA = Not applicable, ND = No data available

TABLE A-1-15

CHEMICAL-SPECIFIC INPUTS FOR ARAMITE (140-57-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	121.75
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	903.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	NA
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.73E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.96E-06
Log K_{ow} (unitless)	U.S. EPA (2000).	4.82
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.47E+04
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.47E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.11E+03
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1995g)	4.00E+01
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g).	7.54E+03

TABLE A-1-15

CHEMICAL-SPECIFIC INPUTS FOR ARAMITE (140-57-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	5.00E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	2.50E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.75E-01
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	2.50E-02
MCL	National Primary Drinking Water Regulations.	6E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.60E+2

Note: NA = Not applicable, ND = No data available

TABLE A-1-16

CHEMICAL-SPECIFIC INPUTS FOR ARSENIC (7440-38-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	74.92
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1,091 at 36 atm
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.07E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.24E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated using the MINTEQ2 geochemical speciation model. The default value used by DRAS is based on the most neutral pH (6.8).	25 at pH=4.9; 29 at pH=6.8; 31 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). The default value used by DRAS is based on the most neutral pH (6.8).	25 at pH=4.9; 29 at pH=6.8; 31 at pH=8.0
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.00E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	ND
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b)	1.14E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-16

CHEMICAL-SPECIFIC INPUTS FOR ARSENIC (7440-38-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.0E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.5E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.5E+01
MCL	National Primary Drinking Water Regulations.	1.0E-02
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	1.50E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-17

CHEMICAL-SPECIFIC INPUTS FOR ATRIZINE (1912-24-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	121.75
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	903.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	NA
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.73E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.96E-06
Log K_{ow} (unitless)	Hansch (1995).	2.61
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.40E+02
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.40E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.05E+01
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980).	5.67E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-17

CHEMICAL-SPECIFIC INPUTS FOR ATRIZINE (1912-24-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.5E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	2.2E-01
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.23E-01
Inhalation CSF $(mg/kg/day)^{-1}$	Route to route extrapolation from Oral CSF.	2.2E-01
MCL	National Primary Drinking Water Regulations.	3.0E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.60E+2

Note: NA = Not applicable, ND = No data available

TABLE A-1-18

CHEMICAL-SPECIFIC INPUTS FOR BARIUM (7440-39-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	137.33
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	983
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.14E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.26E-06
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. The default value used by DRAS is based on the most neutral pH (6.8).	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). The default value used by DRAS is based on the most neutral pH (6.8).	11 at pH=4.9; 41 at pH=6.8; 52 at pH=8.0
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b).	6.33E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-18

CHEMICAL-SPECIFIC INPUTS FOR BARIUM (7440-39-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2005a)	2.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (1997c)	5.0E-04
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	2
Aquatic TRV (ug/l)	U.S. EPA (1996c)	3.9E+00

Note: NA = Not applicable, ND = No data available

TABLE A-1-19

CHEMICAL-SPECIFIC INPUTS FOR BENZALDEHYDE (100-52-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	121.75
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	903.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	NA
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.73E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.96E-06
Log K_{ow} (unitless)	Hansch (1995).	1.48
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.78E+01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.78E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.33E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980).	7.80E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-19

CHEMICAL-SPECIFIC INPUTS FOR BENZALDEHYDE (100-52-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	3.5E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	6E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.60E+2

Note: NA = Not applicable, ND = No data available

TABLE A-1-20

CHEMICAL-SPECIFIC INPUTS FOR BENZENE (71-43-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	78.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	278.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.25E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.78E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.49E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.80E-06
Log K_{ow} (unitless)	Hansch (1995).	2.13
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	6.20E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.20E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.65E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.10E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.60E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	6.30E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.30E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.45E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-20

CHEMICAL-SPECIFIC INPUTS FOR BENZENE (71-43-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	4.00E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	5.5E-02
RfC (mg/m^3)	U.S. EPA (2004b)	3.01E-02
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	2.70E-02
MCL	National Primary Drinking Water Regulations.	5E-03
Aquatic TRV (ug/l)	U.S. EPA (1996c)	4.6E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-21

CHEMICAL-SPECIFIC INPUTS FOR BENZIDINE (92-87-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	184.23
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	390.65
Vp (atm)	--	ND
S (g/2500ml)	Geometric mean value cited in U.S. EPA (1994c).	1.0
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.88E-11
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.50E-05
Log K_{ow} (unitless)	Hansch (1995).	1.34
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.08E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.08E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.56E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.20E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.80E+00
B	*B* value was obtained from U.S. EPA (1992b).	4.60E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	6.14E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-21

CHEMICAL-SPECIFIC INPUTS FOR BENZIDINE (92-87-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.00E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	2.30E+02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.05E-02
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	2.35E+02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1995f)	2.5E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-22

CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)ANTHRACENE (56-55-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	228.28
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	433
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.03E-10 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.28E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	3.62E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	2.47E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	6.21E-06
Log K_{ow} (unitless)	Wang (1986).	5.76
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	2.60E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.60E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.94E+04
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	8.60E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.00E+01
B	*B* value was obtained from U.S. EPA (1992b).	5.00E+01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	5.10E+03

TABLE A-1-22

CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)ANTHRACENE (56-55-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	Calculated by multiplying the *Oral CSF* for Benzo(a)pyrene by the relative potency factor for Benzo(a)anthracene of 0.1 (U.S. EPA 1993b).	7.31E-01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1993b) & Thyssen (1981)	3.10E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Suter (1996)	2.7E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1-23

CHEMICAL-SPECIFIC INPUTS FOR BENZO(B)FLUORANTHENE (205-99-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	252.32
T_m (K)	Montgomery and Welkom (1991)	441
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.06E-10 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	4.33E-03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	6.18E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	2.28E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	5.49E-06
Log K_{ow} (unitless)	Wang (1986).	5.78
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.81E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.81E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.64E+04
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.40E+00
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.00E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.40E+01
B	*B* value was obtained from U.S. EPA (1992b).	1.60E+02

TABLE A-1-23

CHEMICAL-SPECIFIC INPUTS FOR BENZO(B)FLUORANTHENE (205-99-2)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	9.95E+03
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	Calculated by multiplying the *Oral CSF* for Benzo(a)pyrene by the relative potency factor for Benzo(b)fluoranthene of 0.1 (U.S. EPA 1993b).	7.3E-01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1993b) & Thyssen (1981)	3.10E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-24

CHEMICAL-SPECIFIC INPUTS FOR BENZO(K)FLUORANTHENE (207-08-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	252.32
T_m (K)	Montgomery and Welkom (1991)	490
Vp (atm)	U.S. EPA (1994b)	1.32E-12 at 25°C (solid)
S (mg/L)	U.S. EPA (1994b)	8.0E-04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	4.15E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	2.28E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	5.49E-06
Log K_{ow} (unitless)	De Maagd (1998).	6.11
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.01E+06
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.04E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.61E+04
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.00E+00
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.03E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.43E+01
B	*B* value was obtained from U.S. EPA (1992b).	1.00E+02

TABLE A-1-24

CHEMICAL-SPECIFIC INPUTS FOR BENZO(K)FLUORANTHENE (207-08-9)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	9.95E+03
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	Calculated by multiplying the *Oral CSF* for Benzo(a)pyrene by the relative potency factor for benzo(k)fluoranthene of 0.01 (U.S. EPA 1993b)	7.3E-02
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1993b) & Thyssen (1981)	3.10E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-25

CHEMICAL-SPECIFIC INPUTS FOR BENZO(GHI)PERYLENE (191-24-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	276.34
T_m (°K)	--	ND
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	7.40229E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database in U.S. EPA (1994f).	2.01E-02
D_w (cm^2/s)	D_W value was obtained from CHEMDAT8 database in U.S. EPA (1994f).	5.26E-06
Log K_{ow} (unitless)	Hansch (1995).	6.63
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.29E+06
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.29E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.47E+05
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.62E+00
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.24E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.00E+01
B	*B* value was obtained from U.S. EPA (1992b).	3.16E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW_{tissue})	--	ND
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were	1.70E+06

TABLE A-1-25

CHEMICAL-SPECIFIC INPUTS FOR BENZO(GHI)PERYLENE (191-24-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-26

CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)PYRENE (50-32-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	252.3
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	452
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	6.43E-12 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.94E-03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	8.36E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database in U.S. EPA (1994d).	2.18E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database in U.S. EPA (1994d).	5.85E-06
Log K_{ow} (unitless)	De Maagd (1998).	6.13
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	9.69E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.69E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.27E+04
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.20E+00
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.00E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.40E+01
B	*B* value was obtained from U.S. EPA (1992b).	1.30E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	9.95E+03

TABLE A-1-26

CHEMICAL-SPECIFIC INPUTS FOR BENZO(A)PYRENE (50-32-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1993b)	7.30E+00
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1993b) & Thyssen (1981)	7.30E+00
MCL	National Primary Drinking Water Regulations.	2E-04
Aquatic TRV (ug/l)	U.S. EPA (1996c)	1.4E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1-27

CHEMICAL-SPECIFIC INPUTS FOR BENZOIC ACID (7440-36-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	121.75
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	903.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	NA
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.73E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.96E-06
Log K_{ow} (unitless)	Hansch (1995).	1.87
K_{oc} (mL/g)	U.S. EPA (1996a). The default value used by DRAS is based on the most neutral pH (6.8).	5.5 at pH=4.9 0.6 at pH=6.8 0.5 at pH=8.0
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.00E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.50E-02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980).	1.55E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-27

CHEMICAL-SPECIFIC INPUTS FOR BENZOIC ACID (7440-36-0)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	4.0E+00
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.4E+01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	6E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.60E+2

Note: NA = Not applicable, ND = No data available

TABLE A-1-28

CHEMICAL-SPECIFIC INPUTS FOR BENZYL ALCOHOL (100-51-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	108.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	288.29
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.40E-04 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	4.00E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.78E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.89E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.38E-06
Log K_{ow} (unitless)	Hansch (1995).	1.1
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.90E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.90E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.68E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.60E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.00E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	9.60E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.30E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	4.04E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-28

CHEMICAL-SPECIFIC INPUTS FOR BENZYL ALCOHOL (100-51-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2008)	5.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.75E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Suter (1996)	3.75E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-29

CHEMICAL-SPECIFIC INPUTS FOR BENZYL CHLORIDE (100-44-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	126.58
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	225.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.60E-03 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	4.90E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.13E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.43E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.80E-06
Log K_{ow} (unitless)	Hansch (1995).	2.3
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.94E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.94E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.95E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.40E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	5.20E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.20E+00
B	*B* value was obtained from U.S. EPA (1992b).	2.00E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.30E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-29

CHEMICAL-SPECIFIC INPUTS FOR BENZYL CHLORIDE (100-44-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2008)	2.0E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.70E-01
RfC (mg/m^3)	U.S. EPA (2008)	1.0E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-30

CHEMICAL-SPECIFIC INPUTS FOR BERYLLIUM (7440-41-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	9.01
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1,560
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.39E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	5.08E-05
K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. The default value used by DRAS is based on the most neutral pH (6.8).	23 at pH=4.9; 790 at pH=6.8; 1.0E+05 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). The default value used by DRAS is based on the most neutral pH (6.8).	23 at pH=4.9; 790 at pH=6.8; 1.0E+05 at pH=8.0
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b).	6.20E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-30

CHEMICAL-SPECIFIC INPUTS FOR BERYLLIUM (7440-41-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	2.00E-05
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	8.40E+00
MCL	National Primary Drinking Water Regulations.	4.00E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	5.10E+00

Note: NA = Not applicable, ND = No data available

TABLE A-1-31

CHEMICAL-SPECIFIC INPUTS FOR BIS-(2-CHLOROETHOXY) METHANE (111-91-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1990)	173.04
T_m (°K)	Montgomery and Welkom (1990)	240.35
Vp (1mm @53 °C)	Montgomery and Welkom (1990)	1.0
S (mg/L@ 25 °C)	All metals, except mercury, are assumed to be insoluble in water.	81,000.00
H (atm·m^3/mol)	U.S. EPA (1998c)	3.78E-07
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	3.20E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.46E-06
Log K_{ow} (unitless)	Montgomery and Welkom (1990)	1.26
K_{oc} (mL/g)	Montgomery and Welkom (1990)	1.14E+02
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.14E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.55E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	131E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	9.95E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.39E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.82E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-31

CHEMICAL-SPECIFIC INPUTS FOR BIS-(2-CHLOROETHOXY) METHANE (111-91-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-32

CHEMICAL-SPECIFIC INPUTS FOR (BIS)-1,2-CHLOROISOPROPYLETHER (39638-32-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	171.07
T_m (K)	Montgomery and Welkom (1991)	369.9
Vp (atm)	Montgomery and Welkom (1991)	7.00E-03 at 25°C (solid)
S (mg/L)	Montgomery and Welkom (1991)	1.70E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.04E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.61E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.38E-06
Log K_{ow} (unitless)	K_{ow} value cited in Howard (1989 - 1993).	2.58
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.44E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.44E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.58E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.02E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	9.70E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.30E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.80E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	5.38E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-32

CHEMICAL-SPECIFIC INPUTS FOR (BIS)-1,2-CHLOROISOPROPYLETHER (39638-32-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	4.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation [1] *CSF* $(mg/kg/day)^{-}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-33

CHEMICAL-SPECIFIC INPUTS FOR BIS(2-CHLORETHYL)ETHER (111-44-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	143.02
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	223.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.76E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.18E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.13E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.40E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.70E-06
Log K_{ow} (unitless)	Hansch (1995).	1.29
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	7.60E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.60E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.70E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.80E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	6.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.60E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.60E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	5.63E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-33

CHEMICAL-SPECIFIC INPUTS FOR BIS(2-CHLORETHYL)ETHER (111-44-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	1.1E+00
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	1.1E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	2.380E+03

Note: NA = Not applicable, ND = No data available

TABLE A-1-34

CHEMICAL-SPECIFIC INPUTS FOR BIS-(2-ETHYLHEXYL) PHTHALATE (117-81-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	390.54
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	218.1
Vp (atm)	*Vp* value cited in U.S. EPA (1998c).	8.49E-09 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1998c).	3.96E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.37E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.32E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.22E-06
Log K_{ow} (unitless)	DeBruijn (1989).	7.6
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.11E+05
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.11E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.32E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	3.30E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.10E+01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.00E+02
B	*B* value was obtained from U.S. EPA (1992b).	1.30E+01

TABLE A-1-34

CHEMICAL-SPECIFIC INPUTS FOR BIS-(2-ETHYLHEXYL) PHTHALATE (117-81-7)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	3.60E+02
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.00E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.40E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.00E-02
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	1.4E-02
MCL	National Primary Drinking Water Regulations.	6.0E-03
Aquatic TRV (ug/l)	U.S. EPA (1996c)	3.2E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-35

CHEMICAL-SPECIFIC INPUTS FOR BROMODICHLOROMETHANE (75-27-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	163.83
T_m (K)	Montgomery and Welkom (1991)	218.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.68E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.97E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.17E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.98E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.06E-05
Log K_{ow} (unitless)	Sangster (1994).	2.0
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.59E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.59E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.45E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.90E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	8.70E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.10E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.30E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.95E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-35

CHEMICAL-SPECIFIC INPUTS FOR BROMODICHLOROMETHANE (75-27-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.00E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	6.20E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.00E-02
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	6.20E-02
MCL	National Primary Drinking Water Regulations.	8.0E-02 TTHM
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-36

CHEMICAL-SPECIFIC INPUTS FOR BROMOFORM (TRIBROMOMETHANE) (75-25-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	252.77
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	280.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.82E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.21E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.16E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.41E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.03E-05
Log K_{ow} (unitless)	Chem Inspect Test Inst. (1992).	2.4
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.26E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.26E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.45E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.609E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.00E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.30E+00
B	*B* value was obtained from U.S. EPA (1992b).	2.20E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.93E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-36

CHEMICAL-SPECIFIC INPUTS FOR BROMOFORM (TRIBROMOMETHANE) (75-25-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.00E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	7.90E-03
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	3.90E-03
MCL	National Primary Drinking Water Regulations.	8.0E-02 TTHM
Aquatic TRV (ug/l)	U.S. EPA (1995f)	2.93E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-37

CHEMICAL-SPECIFIC INPUTS FOR 4-BROMOPHENYL-PHENYLETHER (101-55-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	249.2
T_m (K)	Montgomery and Welkom (1991)	291.8
Vp (atm)	*Vp* value cited in Montgomery and Welkom (1991).	1.97E-06 at 25°C (liquid)
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.98E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.83E-06
Log K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	5.04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.01E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.01E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.76E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	6.30E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.89E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.63E+01
B	*B* value was obtained from U.S. EPA (1992b).	1.91E+00
Biotransfer Factors for Animals		
BCF_{fish} (unitless FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	1.45E+04

TABLE A-1-37

CHEMICAL-SPECIFIC INPUTS FOR 4-BROMOPHENYL-PHENYLETHER (101-55-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1996c)	1.5E+00

Note: NA = Not applicable, ND = No data available

TABLE A-1-38

CHEMICAL-SPECIFIC INPUTS FOR BUTANOL (71-36-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1995g)	74.12
T_m (K)	--	
Vp (atm)	U.S. EPA (1995g)	8.60E-03
S (mg/L)	U.S. EPA (1995g)	7.50E+04
H (atm·m^3/mol)	U.S. EPA (1995g)	8.81E-06
D_a (cm^2/s)	U.S. EPA (1995g)	8.00E-02
D_w (cm^2/s)	U.S. EPA (1995g)	9.30E-06
Log K_{ow} (unitless)	Hansch (1995).	0.88
K_{oc} (mL/g)	U.S. EPA (1995g)	6.10E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.10E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.58E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.50E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.90E-01
B	*B* value was obtained from U.S. EPA (1992b).	6.30E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.75E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-38

CHEMICAL-SPECIFIC INPUTS FOR BUTANOL (71-36-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-39

CHEMICAL-SPECIFIC INPUTS FOR BUTYL-BENZYL PHTHALATE (85-68-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Howard (1989-1993)	312.39
T_m (K)	Howard (1989-1993)	238.0
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.58E-08 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.58E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.91E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.65E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.17E-06
Log K_{ow} (unitless)	Ellington (1996).	4.73
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.37E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.37E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.03E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	6.50E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	7.00E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.40E+01
B	*B* value was obtained from U.S. EPA (1992b).	6.90E+00
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s	5.68E+03

TABLE A-1-39

CHEMICAL-SPECIFIC INPUTS FOR BUTYL-BENZYL PHTHALATE (85-68-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.00E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1996c)	1.9E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-40

CHEMICAL-SPECIFIC INPUTS FOR BUTYL-4,6-DINITROPHENOL, 2-SEC (DINOSEB) (88-85-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	240.22
T_m (K)	U.S. EPA (1995b)	311.15 to 414.15
Vp (atm)	U.S. EPA (1995g)	9.90E-05
S (mg/L)	U.S. EPA (1995g)	5.20E+01
H (atm·m^3/mol)	U.S. EPA (1995g)	4.56E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	3.56
K_{oc} (mL/g)	U.S. EPA (1995g)	1.20E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.20E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.00E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.60E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.30E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.40E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.96E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-40

CHEMICAL-SPECIFIC INPUTS FOR BUTYL-4,6-DINITROPHENOL, 2-SEC (DINOSEB) (88-85-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	3.50E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	7.0E-03
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-41

CHEMICAL-SPECIFIC INPUTS FOR CADMIUM (7440-43-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	112.41
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	594.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	8.16E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	9.45E-06
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. The default value used by DRAS is based on the most neutral pH (6.8).	15 at pH=4.9; 75 at pH=6.8; 4.3E+03 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). The default value used by DRAS is based on the most neutral pH (6.8).	15 at pH=4.9; 75 at pH=6.8; 4.3E+03 at pH=8.0
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b).	9.07E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-41

CHEMICAL-SPECIFIC INPUTS FOR CADMIUM (7440-43-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	6.3E+00
MCL	National Primary Drinking Water Regulations.	5E-03
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	2.2E+00

Note: NA = Not applicable, ND = No data available

TABLE A-1-42

CHEMICAL-SPECIFIC INPUTS FOR CARBON DISULFIDE (75-15-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	76.14
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	161.5
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.47E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.67E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.27E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.04E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.29E-05
Log K_{ow} (unitless)	Hansch (1995).	1.94
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.12E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.12E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.09E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.70E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	6.10E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.00E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.76E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-42

CHEMICAL-SPECIFIC INPUTS FOR CARBON DISULFIDE (75-15-0)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	7.00E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Suter (1996)	1E+03

Note: NA = Not applicable, ND = No data available

TABLE A-1-43

CHEMICAL-SPECIFIC INPUTS FOR CARBON TETRACHLORIDE (56-23-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	153.84
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	250.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.48E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.92E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S*, and *Vp* values that are provided in this table.	2.87E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.56E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.77E-06
Log K_{ow} (unitless)	Hansch (1995).	2.83
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	1.52E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.52E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.14E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.90E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	7.60E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.80E+00
B	*B* value was obtained from U.S. EPA (1992b).	5.40E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)	3.00E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-43

CHEMICAL-SPECIFIC INPUTS FOR CARBON TETRACHLORIDE (56-23-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	7.00E-04
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	1.30E-01
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	5.25E-02
MCL	National Primary Drinking Water Regulations.	5E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	3.52E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-44

CHEMICAL-SPECIFIC INPUTS FOR CHLORDANE (57-74-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	409.80
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	381.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.55E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.51E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.64E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.18E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.37E-06
Log K_{ow} (unitless)	Simpson (1995).	6.16
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	5.13E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.13E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.85E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.90E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.80E+01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.30E+02
B	*B* value was obtained from U.S. EPA (1992b).	2.10E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAF*s were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	5.63E+05

TABLE A-1-44

CHEMICAL-SPECIFIC INPUTS FOR CHLORDANE (57-74-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.00E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	3.50E-01
RfC (mg/m^3)	U.S. EPA (2004b)	7.00E-04
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	3.50E-01
MCL	National Primary Drinking Water Regulations.	2E-03
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	4.3E--03

Note: NA = Not applicable, ND = No data available

TABLE A-1-45

CHEMICAL-SPECIFIC INPUTS FOR CHLORINE (7782-50-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	71.90
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	172.1
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	--	1.10E-01
D_w (cm^2/s)	--	1.27E-05
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	ND
ô (hr)	ô value was obtained from U.S. EPA (1992b).	ND
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW)	--	NA
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-45

CHEMICAL-SPECIFIC INPUTS FOR CHLORINE (7782-50-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	CalEPA (2000)	2.0E-04
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	4E+00 MRDL
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-46

CHEMICAL-SPECIFIC INPUTS FOR CHLOROANILINE, p- (106-47-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	121.75
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	903.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	NA
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.73E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.96E-06
Log K_{ow} (unitless)	Hansch (1995).	1.83
K_{oc} (mL/g)	--	6.00E-01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.00E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.50E-02
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.45E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-46

CHEMICAL-SPECIFIC INPUTS FOR CHLOROANILINE, p- (106-47-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	4.0E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2008)	2.0E-01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	6E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.60E+2

Note: NA = Not applicable, ND = No data available

TABLE A-1-47

CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZENE (108-90-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	112.56
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	228.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.59E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.09E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.38E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.35E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.49E-06
Log K_{ow} (unitless)	Sangster (1994).	2.84
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.24E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.24E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.68E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	4.20E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.30E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	7.20E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	8.48E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-47

CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZENE (108-90-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004c)	5.0E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	1E-01
Aquatic TRV (ug/l)	U.S. EPA (1996c)	1.3E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-48

CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZILATE (510-15-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	325.20
T_m (K)	Howard (1989-1993)	309.0
Vp (atm)	Howard (1989-1993)	2.90E-09 at 25°C (solid)
S (mg/L)	Howard (1989-1993)	1.30E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.24E-08
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	1.65E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	4.72E-06
Log K_{ow} (unitless)	Chem Inspect Test Inst (1992).	4.74
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.57E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.57E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.43E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.50E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	8.40E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	2.40E+00
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAF*s were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Carroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	5.78E+03

TABLE A-1-48

CHEMICAL-SPECIFIC INPUTS FOR CHLOROBENZILATE (510-15-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.0E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	2.7E-01
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.0E-02
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	2.7E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-49

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORO-1,3-BUTADIENE (CHLOROPRENE) (126-99-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1995g)	88.54
T_m (K)	--	
Vp (atm)	U.S. EPA (1995g)	2.80E-01
S (mg/L)	U.S. EPA (1995g)	6.30E+02
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.04E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.00E-05
Log K_{ow} (unitless)	U.S. EPA (1995g)	2.08
K_{oc} (mL/g)	U.S. EPA (1995g)	1.10E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table. 5g)	1.10E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.25E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.60E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.00E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.30E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.20E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.24E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-49

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORO-1,3-BUTADIENE (CHLOROPRENE) (126-99-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	7.00E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-51

CHEMICAL-SPECIFIC INPUTS FOR CHLORODIFLUOROMETHANE (75-45-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Howard 1989-1993	86.47
T_m (K)	Howard 1989-1993	126.6
Vp (atm)	*Vp* value cited in Howard 1989-1993.	5.63E+00 at 25°C (liquid)
S (mg/L)	Howard 1989-1993	2.90E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.68E-01
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	9.72E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.13E-05
Log K_{ow} (unitless)	Hansch (1995).	1.08
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.58E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.58E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.44E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	ND
ô (hr)	ô value was obtained from U.S. EPA (1992b).	ND
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.90E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-51

CHEMICAL-SPECIFIC INPUTS FOR CHLORODIFLUOROMETHANE (75-45-6)

Parameter	Reference and Explanation	Value
Health Benchmark		
RfD (mg/kg/day)	Calculated from *RfC* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.40E+01
Oral CSF $(mg/kg/day)^{-1}$		ND
RfC (mg/m^3)	U.S. EPA (2004b)	4.9+01
Inhalation CSF $(mg/kg/day)^{-1}$		ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-52

CHEMICAL-SPECIFIC INPUTS FOR CHLOROETHANE (75-00-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	64.52
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	441.8
Vp (atm)	*Vp* value cited in Lucius et al. (1992).	1.60E+02 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1994a)	5.74E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.80
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.27E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.53E-06
Log K_{ow} (unitless)	Hansch (1995)..	1.43
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.62E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.62E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.22E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	7.19E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-52

CHEMICAL-SPECIFIC INPUTS FOR CHLOROETHANE (75-00-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997a)	4.00E-01
Oral CSF $(mg/kg/day)^{-1}$		ND
RfC (mg/m^3)	U.S. EPA (2004b)	1.00E+01
Inhalation CSF $(mg/kg/day)^{-1}$		ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-53

CHEMICAL-SPECIFIC INPUTS FOR CHLOROFORM (TRICHLOROMETHANE) (67-66-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	119.39
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	209.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.69E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.96E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.03E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.17E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.09E-05
Log K_{ow} (unitless)	Hansch (1995).	1.97
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	5.30E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.30E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.98E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	8.30E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.70E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.10E+00
B	*B* value was obtained from U.S. EPA (1992b).	8.30E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)	3.59E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-53

CHEMICAL-SPECIFIC INPUTS FOR CHLOROFORM (TRICHLOROMETHANE) (67-66-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	ATSDR (1997)	9.93E-02
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	8.10E-02
MCL	National Primary Drinking Water Regulations.	8.0E-02 TTHM
Aquatic TRV (ug/l)	U.S. EPA (1995f)	2.89+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-54

CHEMICAL-SPECIFIC INPUTS FOR 4-CHLORO-3-METHYLPHENOL (59-50-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	142.58
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	328.6
Vp (atm)	U.S. EPA (1998c)	1.08E-05
S (mg/L)	U.S. EPA (1998c)	3.85E+03
H (atm·m^3/mol)	U.S. EPA (1998c)	4.00E-07
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	6.96E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.06E-06
Log K_{ow} (unitless)	Hansch (1995).	3.1
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.41E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.41E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.56E+01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	4.09E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	6.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	1.26E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.34E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-54

CHEMICAL-SPECIFIC INPUTS FOR 4-CHLORO-3-METHYLPHENOL (59-50-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-55

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORONAPHTHALENE (91-58-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	127.57
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	345.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.09E-05 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.36E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.17E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.02E-05
Log K_{ow} (unitless)	Hansch (1995).	4.14
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	K_{oc} is 41 for pH range of 4.9 to 8
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.06E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.05E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	6.50E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	5.20E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.30E+00
B	*B* value was obtained from U.S. EPA (1992b).	7.10E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg $_{FW\ tissue}$)	--	NA

TABLE A-1-55

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORONAPHTHALENE (91-58-7)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	*BAF*s were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	1.14E+03

TABLE A-1-55

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLORONAPHTHALENE (91-58-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	8.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-56

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLOROPHENOL (95-57-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	128.56
T_m (K)	Montgomery and Welkom (1991)	282.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.77E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.15E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.66E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.01E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.46E-06
Log K_{ow} (unitless)	Hansch (1995).	2.15
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1-4 398.0 5 397.9 6 396.9 7 387.3 8 311.8 9 108.7 10 19.43 11 7.39 12 6.14 13 6.01 14 6.00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	3.87E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.90E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.10E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	5.30E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.30E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.40E-02

TABLE A-1-56

CHEMICAL-SPECIFIC INPUTS FOR 2-CHLOROPHENOL (95-57-8)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.54E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1996c)	4.4E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-57

CHEMICAL-SPECIFIC INPUTS FOR 4-CHLOROPHENYL-PHENYLETHER (7005-72-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	204.66
T_m (K)	Montgomery and Welkom (1991)	265.1
Vp (atm)	*Vp* value cited in Montgomery and Welkom (1991).	3.55E-06 at 25°C (liquid)
S (mg/L)	*S* value cited in Montgomery and Welkom (1991).	3.30E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.20E-04
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	3.82E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.42E-06
Log K_{ow} (unitless)	Kurz (1999).	4.7
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.31E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.31E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.74E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND

TABLE A-1-57

CHEMICAL-SPECIFIC INPUTS FOR 4-CHLOROPHENYL-PHENYLETHER (7005-72-3)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	4.78E+03
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-58

CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM (Mixture of Cr(+3) and Cr(+6)) (7440-47-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	52
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	2,173.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database in U.S. EPA (1994f).	1.01E-01
D_w (cm^2/s)	D_W value was obtained from CHEMDAT8 database in U.S. EPA (1994f).	4.63E-05
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. The default value used by DRAS is based on the most neutral pH (6.8).	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). The default value used by DRAS is based on the most neutral pH (6.8).	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b).	1.90E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-58

CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM (Mixture of Cr(+3) and Cr(+6)) (7440-47-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b) for Chromium (+6).	3.0E+-3
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b) as a mixture of Cr (+3) and Cr(+6)	4.2E+01
MCL	National Primary Drinking Water Regulations.	1E-01
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	7.4E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-59

CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM (+3) (16065-38-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	51.996
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	2173.15
Vp (atm)	--	0
S (mg/L)	--	0
H (atm·m^3/mol)	--	0
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.01E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	4.63E-05
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. The default value used by DRAS is based on the most neutral pH (6.8).	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). The default value used by DRAS is based on the most neutral pH (6.8).	1.2E+03 at pH=4.9; 1.8E+06 at pH=6.8; 4.3E+06 at pH=8.0
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	ND
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b).	1.90E+01
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-59

CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM (+3) (16065-38-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.5E+00
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	1.0E-01
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-60

CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM HEXAVALENT (18540-29-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	52
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	2,173.0
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.36E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.58E-05
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. The default value used by DRAS is based on the most neutral pH (6.8).	31 at pH=4.9; 19 at pH=6.8; 14 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). The default value used by DRAS is based on the most neutral pH (6.8).	31 at pH=4.9; 19 at pH=6.8; 14 at pH=8.0
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b).	1.90E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-60

CHEMICAL-SPECIFIC INPUTS FOR CHROMIUM HEXAVALENT (18540-29-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b) for Chromium (+6).	3.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b) for Chromium (+6).	1.00E-04
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b) for Chromium (+6) adjusted for the proportion of Cr(+6) in the original study (1 part in 7).	2.94E+02
MCL	National Primary Drinking Water Regulations.	1.0E-01
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	1.10E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-61

CHEMICAL-SPECIFIC INPUTS FOR CHRYSENE (218-01-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	228.28
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	527.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.03E-11 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.94E-03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	1.21E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	2.48E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	6.21E-06
Log K_{ow} (unitless)	De Maagd (1998).	5.81
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.15E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.15E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.86E+04
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	8.60E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.00E+01
B	*B* value was obtained from U.S. EPA (1992b).	5.00E+01

TABLE A-1-61

CHEMICAL-SPECIFIC INPUTS FOR CHRYSENE (218-01-9)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	6.03E+03
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	Calculated by multiplying the *Oral CSF* for Benzo(a)pyrene by the relative potency factor for chrysene of 0.001 (U.S. EPA 1993b)	7.30E-03
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1993b) and Thyssen (1981).	3.10E-03
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-62

CHEMICAL-SPECIFIC INPUTS FOR CIS-1,3-DICHLOROPROPENE (10061-01-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	110.97
T_m (°K)	--	
Vp (atm)	U.S. EPA (1995g)	4.99E-02
S (mg/L)	U.S. EPA (1995g)	2.70E+03
H (atm·m^3/mol)	U.S. EPA (1995g)	1.76E-03
D_a (cm^2/s)	U.S. EPA (1995g)	5.85E-02
D_w (cm^2/s)	U.S. EPA (1995g)	1.10E-05
Log K_{ow} (unitless)	Tomlin (1997)	2.06
K_{oc} (mL/g)	U.S. EPA (1995g)	9.30E+01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.30E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.97E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.20E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.00E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.17E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-62

CHEMICAL-SPECIFIC INPUTS FOR CIS-1,3-DICHLOROPROPENE (10061-01-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b) for mixture of cis- and trans-1,3-dichloropropene	3.0E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b) for mixture of cis- and trans-1,3-dichloropropene	1.0E-01
RfC (mg/m^3)	U.S. EPA (2004b) for mixture of cis- and trans-1,3-dichloropropene	2.0E-02
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b) for mixture of cis- and trans-1,3-dichloropropene	1.4E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1995f)	2.40E+01

Note: Not applicable, ND = No data available

TABLE A-1-63

CHEMICAL-SPECIFIC INPUTS FOR COBALT (7440-48-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	58.93
T_m (K)	Montgomery and Welkom (1991)	1766.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	--	NA
D_w (cm^2/s)	--	NA
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	ND
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-63

CHEMICAL-SPECIFIC INPUTS FOR COBALT (7440-48-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2008)	3.0E-4
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2008)	6.0E-06
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2008)	3.15E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-64

CHEMICAL-SPECIFIC INPUTS FOR COPPER (744-050-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	63.55
T_m (K)	Montgomery and Welkom (1991)	1356.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	--	NA
D_w (cm^2/s)	--	NA
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	2.20E+01
Kd_{sw} (L/Kg)	--	2.20E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	ND
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	U.S. EPA (1998b).	7.10E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-64

CHEMICAL-SPECIFIC INPUTS FOR COPPER (744-050-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	4.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	1.3
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	9.00E+00

Note: NA = Not applicable, ND = No data available

TABLE A-1-65

CHEMICAL-SPECIFIC INPUTS FOR M-CRESOL (108-39-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	108.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	284.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.90E-04 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	2.30E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.93E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.93E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.30E-06
Log K_{ow} (unitless)	Hansch (1995).	1.96
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.45E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.45E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.34E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.00E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.00E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	9.60E-01
B	*B* value was obtained from U.S. EPA (1992b).	9.30E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.82E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-65

CHEMICAL-SPECIFIC INPUTS FOR M-CRESOL (108-39-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-66

CHEMICAL-SPECIFIC INPUTS FOR O-CRESOL (95-48-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	108.13
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	303.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.16E-04 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.77E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.62E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.88E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.41E-06
Log K_{ow} (unitless)	Hansch (1995).	1.95
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.26E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.26E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.20E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.10E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.00E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	9.60E-01
B	*B* value was obtained from U.S. EPA (1992b).	9.80E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.79E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-66

CHEMICAL-SPECIFIC INPUTS FOR O-CRESOL (95-48-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-67

CHEMICAL-SPECIFIC INPUTS FOR P-CRESOL (106-44-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	108.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	308.6
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.70E-04 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	2.30E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.99E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.93E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.30E-06
Log K_{ow} (unitless)	Hansch (1995).	1.94
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.08E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.08E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.20E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.00E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.00E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	9.60E-01
B	*B* value was obtained from U.S. EPA (1992b).	8.90E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.76E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-67

CHEMICAL-SPECIFIC INPUTS FOR P-CRESOL (106-44-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	5.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-68

CHEMICAL-SPECIFIC INPUTS FOR CUMENE (ISOPROPYLBENZENE) (98-82-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	120.19
T_m (K)	U.S. EPA (1995g)	177
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	6.00E-03 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	5.60E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.29E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.50E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.83E-06
Log K_{ow} (unitless)	Hansch (1995).	3.66
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.48E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.48E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.11E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.20E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.70E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.80E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.80E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.56E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-68

CHEMICAL-SPECIFIC INPUTS FOR CUMENE (ISOPROPYLBENZENE) (98-82-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	NA
RfC (mg/m^3)	U.S. EPA (2004b)	3.85E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	NA
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-69

CHEMICAL-SPECIFIC INPUTS FOR CYANIDE (57-12-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1992a)	26.017
T_m (K)	--	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.82E-02 at 25°C (solid)
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	5.48E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	2.10E-05
Log K_{ow} (unitless)	Hansch (1995).	-0.25
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	U.S. EPA (1996a).	9.9
Kd_{sw} (L/Kg)	U.S. EPA (1996a).	9.9
Dermal Exposure Factors		
$K_p^{\ w}$ (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b)	6.33E+02
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-69

CHEMICAL-SPECIFIC INPUTS FOR CYANIDE (57-12-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.0E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	2E-01
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	5.2E+00

Note: NA = Not applicable, ND = No data available

TABLE A-1-70

CHEMICAL-SPECIFIC INPUTS FOR CYCLOTETRAMETHYLENETETRANITRAMINE (HMX) (2691-41-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	296.16
T_m (K)	CRC Handbook (1995)	559.15
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from WATER8 model database (U.S. EPA 1995d).	2.60E-15
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	8.00E-06
Log K_{ow} (unitless)	Monteil-Rivera (2003).	0.16
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.28E-05
ô (hr)	ô value was obtained from U.S. EPA (1992b).	6.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-70

CHEMICAL-SPECIFIC INPUTS FOR CYCLOTETRAMETHYLENETETRANITRAMINE (HMX) (2691-41-0)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.75E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-71

CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDD (72-54-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	320.05
T_m (K)	Montgomery and Welkom (1991)	380.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.14E-09 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.33E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.98E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.76E-06
Log K_{ow} (unitless)	Sangster (1994).	6.02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.58E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.58E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.44E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	4.60E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	7.80E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.70E+01
B	*B* value was obtained from U.S. EPA (1992b).	1.30E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	3.94E+05

TABLE A-1-71

CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDD (72-54-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	2.40E-01
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	2.40E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	6.4E-03

Note: NA = Not applicable, ND = No data available

TABLE A-1-72

CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDE (72-55-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	319.03
T_m (K)	Montgomery and Welkom (1991)	361.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.45E-09 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.92E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.24E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.70E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.78E-06
Log K_{ow} (unitless)	Sangster (1993).	6.51
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	8.64E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.64E+06
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.48E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.40E+00
ô (hr)	ô value was obtained from U.S. EPA (1992b).	7.60E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.60E+01
B	*B* value was obtained from U.S. EPA (1992b).	5.80E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	5.53E+05

TABLE A-1-72

CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDE (72-55-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	3.40E-01
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.05E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-73

CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDT (50-29-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	354.49
T_m (K)	Montgomery and Welkom (1991)	381.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.17E-10 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.41E-03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.37E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.48E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.48E-06
Log K_{ow} (unitless)	Hansch (1995).	6.91
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	6.78E+05
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.78E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.08E+04
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.70E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.30E+01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	6.00E+01
B	*B* value was obtained from U.S. EPA (1992b).	3.40E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	2.76E+06

TABLE A-1-73

CHEMICAL-SPECIFIC INPUTS FOR 4,4'-DDT (50-29-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.00E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	3.40E-01
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.75E-03
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	3.40E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	1.0E-03

Note: NA = Not applicable, ND = No data available

TABLE A-1-74

CHEMICAL-SPECIFIC INPUTS FOR DIALLATE (2303-16-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	270.24
T_m (K)	--	ND
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	2.00E-07
S (ppm)	*S* value cited in U.S. EPA (1995b).	40
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.83E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Ellington (1988).	4.49
K_{oc} (mL/g)	Value cited in U.S. EPA (1995g).	2.60E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.60E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.82E+03
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	6.60E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.90E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.00E+01
B	*B* value was obtained from U.S. EPA (1992b).	3.10E+00
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	2.69E+03

TABLE A-1-74

CHEMICAL-SPECIFIC INPUTS FOR DIALLATE (2303-16-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	6.10E-02
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	6.10E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-75

CHEMICAL-SPECIFIC INPUTS FOR DIAZINON (333-41-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	278.33
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	539.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.70E-14 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	6.70E-04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	1.12E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	1.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	6.01E-06
Log K_{ow} (unitless)	Hansch (1995).	3.81
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.57E+03
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.57E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.17E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.10E+00
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.40E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.10E+01
B	*B* value was obtained from U.S. EPA (1992b).	4.90E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	463.02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-75

CHEMICAL-SPECIFIC INPUTS FOR DIAZINON (333-41-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	9.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	3.15E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-76

CHEMICAL-SPECIFIC INPUTS FOR DIBENZ (A,H) ANTHRACENE (53-70-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	278.33
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	539.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.70E-14 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	6.70E-04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S* and *Vp* values that are provided in this table.	1.12E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	1.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	6.01E-06
Log K_{ow} (unitless)	Sangster (1993).	6.75
K_{oc} (mL/g)	Geometric mean of measured values was obtained from U.S. EPA (1996b).	1.79E+06
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.79E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.34E+05
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.10E+00
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.40E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.10E+01
B	*B* value was obtained from U.S. EPA (1992b).	4.90E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	1.28E+04

TABLE A-1-76

CHEMICAL-SPECIFIC INPUTS FOR DIBENZ (A,H) ANTHRACENE (53-70-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	Calculated by multiplying the Oral CSF for Benzo(a)pyrene by the relative potency factor for Dibenz(a,h)anthracene of 1.0 (U.S. EPA 1993b).	7.30E+00
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (1993b) and Thyssen (1981)	3.1E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-77

CHEMICAL-SPECIFIC INPUTS FOR DIBENZOFURAN (132-64-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	168.19
T_m (K)	CRC Handbook (1995)	359.65
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.056E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	4.12
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.06E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	6.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	2.04E+00
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-77

CHEMICAL-SPECIFIC INPUTS FOR DIBENZOFURAN (132-64-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2007)	1.0E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	3.5E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1996c)	2.00E+1

Note: NA = Not applicable, ND = No data available

TABLE A-1-78

CHEMICAL-SPECIFIC INPUTS FOR DIBROMOCHLOROMETHANE (124-48-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	208.3
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	252.1
Vp (atm)	*Vp* value cited in Montgomery and Weldom (1991).	2.00E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	3.44E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.21E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.96E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.05E-05
Log K_{ow} (unitless)	Sangster (1994).	2.16
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.15E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.15E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.61E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	3.50E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.60E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.90E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.50E-02

TABLE A-1-78

CHEMICAL-SPECIFIC INPUTS FOR DIBROMOCHLOROMETHANE (124-48-1)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.58E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.00E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	8.40E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.00E-02
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	8.4E-02
MCL	National Primary Drinking Water Regulations.	8.0E-02 TTHM
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-79

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIBROMO-3-CHLOROPROPANE (96-12-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	236.36
T_m (K)	Montgomery and Welkom (1991)	279.2
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.0E-03 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.20E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.97E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.79E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.79E-06
Log K_{ow} (unitless)	Chemical Inspect Test Inst. (1992).	2.96
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.64E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.64E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.98E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	3.20E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.40E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.80E+00
B	*B* value was obtained from U.S. EPA (1992b).	2.20E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.05E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-79

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIBROMO-3-CHLOROPROPANE (96-12-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2008)	2.0E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2008)	8.0E-01
RfC (mg/m^3)	U.S. EPA (2004b)	2.00E-04
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2008)	2.1E+01
MCL	National Primary Drinking Water Regulations.	2E-04
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-80

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROBENZENE (95-50-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	147.01
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	256.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.79E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.25E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.11E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.11E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.93E-06
Log K_{ow} (unitless)	Hansch (1995).	3.43
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	3.79E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.79E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.84E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	6.60E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	6.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.40E+00
B	*B* value was obtained from U.S. EPA (1992b).	2.70E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.38E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-80

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROBENZENE (95-50-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	9.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (1997c)	2.00E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	6.0E-01
Aquatic TRV (ug/l)	U.S. EPA (1996c)	1.4E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-81

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROBENZENE (541-73-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	147.01
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	297.86
Vp (atm)	*Vp* value cited in Howard (1989-1993).	3.03E-03 at 25°C (solid)
S (mg/L)	*S* value cited in Howard (1989-1993).	6.88E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.11E+02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.14E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.85E-06
Log K_{ow} (unitless)	Hansch (1995).	3.53
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.48E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.48E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.61E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	8.70E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	6.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.10E+00
B	*B* value was obtained from U.S. EPA (1992b).	4.00E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.84E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-81

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROBENZENE (541-73-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1996c)	7.1E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-82

CHEMICAL-SPECIFIC INPUTS FOR 1,4-DICHLOROBENZENE (106-46-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	147.01
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	326.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.39E-03 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.30E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.80E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.14E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.85E-06
Log K_{ow} (unitless)	Hansch (1995).	3.44
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	6.16E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.16E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.62E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	6.50E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	6.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.40E+00
B	*B* value was obtained from U.S. EPA (1992b).	2.60E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.42E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-82

CHEMICAL-SPECIFIC INPUTS FOR 1,4-DICHLOROBENZENE (106-46-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	2.40E-02
RfC (mg/m^3)	U.S. EPA (2004b)	8.05E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	7.5E-02
Aquatic TRV (ug/l)	U.S. EPA (1996c)	1.5E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-83

CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DICHLOROBENZIDINE (91-94-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	253.13
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	405.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.89E-10 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.52E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.08E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.28E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.48E-06
Log K_{ow} (unitless)	Hansch (1995).	3.51
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.21E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.21E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.41E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.70E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.10E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.70E+01
B	*B* value was obtained from U.S. EPA (1992b).	3.20E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.74E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-83

CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DICHLOROBENZIDINE (91-94-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	NA
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	4.50E-01
RfC (mg/m^3)	--	NA
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-84

CHEMICAL-SPECIFIC INPUTS FOR DICHLORODIFLUOROMETHANE (75-71-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	120.92
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	115.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	6.40E+00 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	3.0E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.58E+00
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.77E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	9.00E-06
Log K_{ow} (unitless)	Hansch (1995).	2.16
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.15E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.15E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.61E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.20E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.80E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.10E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.40E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.58E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-84

CHEMICAL-SPECIFIC INPUTS FOR DICHLORODIFLUOROMETHANE (75-71-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (1997c)	2.00E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-85

CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHANE (75-34-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	98.97
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	175.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.0E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.16E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.75E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.42E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.05E-05
Log K_{ow} (unitless)	Hansch (1995).	1.79
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	5.30E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.30E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.98E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	8.90E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.40E-01
B	*B* value was obtained from U.S. EPA (1992b).	6.20E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.35E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-85

CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHANE (75-34-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2008)	2.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (1997c)	5.00E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.58E+03

Note: NA = Not applicable, ND = No data available

TABLE A-1-86

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROETHANE (ETHYLENE DICHLORIDE) (107-06-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	98.96
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	233.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.07E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	8.31E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.27E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.19E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-05
Log K_{ow} (unitless)	Hansch (1995).	1.48
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.96E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.96E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.47E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.20E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.40E-01
B	*B* value was obtained from U.S. EPA (1992b).	3.00E-03
Biotransfer Factors for Animals		
BCF_{fish} (L//kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	7.85E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-86

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROETHANE (ETHYLENE DICHLORIDE) (107-06-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004c)	2.0E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	9.10E-02
RfC (mg/m^3)	ATSDR (2001)	2.47E+00
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	9.28E-02
MCL	National Primary Drinking Water Regulations.	5E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	2.0E+03

Note: NA = Not applicable, ND = No data available

TABLE A-1-87

CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHYLENE (75-35-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	96.95
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	150.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.88E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.0E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.55E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.53E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.09E-05
Log K_{ow} (unitless)	Hansch (1995).	2.13
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	6.50E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.50E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.73E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.00E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.40E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.20E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.30E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.48E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-87

CHEMICAL-SPECIFIC INPUTS FOR 1,1-DICHLOROETHYLENE (75-35-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	2.0E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	7E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	3.03E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-88

CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,2-DICHLOROETHYLENE (156-59-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Howard (1989-1993)	96.94
T_m (K)	Howard (1989-1993)	192.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.30E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.94E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.51E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.36E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.13E-05
Log K_{ow} (unitless)	Hansch (1995).	1.86
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.56E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.56E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.67E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.40E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.40E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.20E-01
B	*B* value was obtained from U.S. EPA (1992b).	7.20E-03
Biotransfer Factors for Animals		
BCF_{fish} (unitless, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.53E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-88

CHEMICAL-SPECIFIC INPUTS FOR (CIS)-1,2-DICHLOROETHYLENE (156-59-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004c)	1.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	7E-02
Aquatic TRV (ug/l)	Suter (1996)	5.72E+03

Note: NA = Not applicable, ND = No data available

TABLE A-1-89

CHEMICAL-SPECIFIC INPUTS FOR (TRANS)-1,2-DICHLOROETHYLENE (156-60-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	96.95
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	223.7
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	4.63E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	6.03E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.44E-03
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	8.16E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	9.75E-06
Log K_{ow} (unitless)	Hansch (1995).	2.09
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	3.80E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.80E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.85E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.40E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.40E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.20E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.20E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.28E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-89

CHEMICAL-SPECIFIC INPUTS FOR (TRANS)-1,2-DICHLOROETHYLENE (156-60-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2008)	6.0E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	1E-01
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.4E+03

Note: NA = Not applicable, ND = No data available

TABLE A-1-90

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOL (120-83-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	163.01
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	318.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	7.21E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	4.93E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.38E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.79E-06
Log K_{ow} (unitless)	Hansch (1995).	3.06
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1-4 159.0 5 158.8 6 156.8 7 139.6 8 67.31 9 12.75 10 3.50 11 2.51 12 2.41 13-14 2.40
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.40E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.05E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	3.00E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	8.60E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.50E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.20E-01

TABLE A-1-90

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOL (120-83-2)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.25E+02
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.0E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	3.6E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-91

CHEMICAL-SPECIFIC INPUTS FOR 2,6-DICHLOROPHENOL (87-65-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	163.01
T_m (K)	Howard (1989-1993)	337.65 to 338.65
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.96E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.47E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.77E-06
Log K_{ow} (unitless)	Hansch (1995).	2.75
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.07E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	8.63E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.07E+00
B	*B* value was obtained from U.S. EPA (1992b).	7.24E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-91

CHEMICAL-SPECIFIC INPUTS FOR 2,6-DICHLOROPHENOL (87-65-0)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-92

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOXYACETIC ACID (94-75-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1995g)	221.04
T_m (K)	--	ND
Vp (atm)	U.S. EPA (1995g)	1.40E-05
S (mg/L)	U.S. EPA (1995g)	6.80E+02
H (atm·m^3/mol)	U.S. EPA (1995g)	4.50E-06
D_a (cm^2/s)	U.S. EPA (1995g)	5.88E-02
D_w (cm^2/s)	U.S. EPA (1995g)	6.49E-06
Log K_{ow} (unitless)	Hansch (1995).	2.81
K_{oc} (mL/g)	U.S. EPA (1995g)	4.50E+02
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.--	4.50E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.37E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	7.10E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.00E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.70E+00
B	*B* value was obtained from U.S. EPA (1992b).	5.00E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	8.05E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-92

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DICHLOROPHENOXYACETIC ACID (94-75-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	3.50E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	7.0E-02
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-93

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROPROPANE (78-87-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	112.99
T_m (K)	Montgomery and Welkom (1991)	172.7
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	6.66E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.68E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.81E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.21E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.71E-06
Log K_{ow} (unitless)	Sangster (1994).	1.98
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.70E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.70E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.53E+00
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	9.80E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.30E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	9.30E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were obtained from U.S. EPA (1995g).	3.02E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-93

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DICHLOROPROPANE (78-87-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c))	6.80E-02
RfC (mg/m^3)	U.S. EPA (2004b)	4.00E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	5.0E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	5.25E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-94

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROPROPENE (542-75-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	110.98
T_m (K)	Montgomery and Welkom (1991)	189.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.11E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.55E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.94E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.26E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.00E-05
Log K_{ow} (unitless)	Tomlin (1997).	2.03
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.70E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.70E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.03E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.10E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.20E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.00E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.05E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-94

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROPROPENE (542-75-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.00E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.00E-01
RfC (mg/m^3)	U.S. EPA (2004b)	2.00E-02
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.40E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Suter (1996)	4.00E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-96

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROPROPENE-TRANS (10061-02-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	110.98
T_m (K)	--	
Vp (atm)	U.S. EPA (1995g)	4.00E-02
S (mg/L)	U.S. EPA (1995g)	2.80E+03
H (atm·m^3/mol)	U.S. EPA (1995g)	1.25E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.85E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-05
Log K_{ow} (unitless)	Tomlin (1997).	2.03
K_{oc} (mL/g)	U.S. EPA (1995g)	9.30E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.30E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.97E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.20E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.00E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.05E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-96

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DICHLOROPROPENE-TRANS (10061-02-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.0E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.0E-01
RfC (mg/m^3)	U.S. EPA (2004b)	2.0E-02
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.4E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1995f)	2.40E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-97

CHEMICAL-SPECIFIC INPUTS FOR DICHLORVOS (62-73-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	110.98
T_m (K)	--	
Vp (atm)	U.S. EPA (1995g)	4.00E-02
S (mg/L)	U.S. EPA (1995g)	2.80E+03
H (atm·m^3/mol)	U.S. EPA (1995g)	1.25E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.85E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-05
Log K_{ow} (unitless)	Bowman (1983).	1.47
K_{oc} (mL/g)	U.S. EPA (1995g)	9.30E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.30E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.97E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.20E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.00E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	7.71E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-97

CHEMICAL-SPECIFIC INPUTS FOR DICHLORVOS (62-73-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.0E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	2.9E-01
RfC (mg/m^3)	U.S. EPA (2004b)	5.0E-04
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	2.9E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1995f)	2.40E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-98

CHEMICAL-SPECIFIC INPUTS FOR DIELDRIN (60-57-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	380.93
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	449.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a)	1.31E-09 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a)	1.87E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.66E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.36E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	4.29E-06
Log K_{ow} (unitless)	DeBruijn (1989).	5.4
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.55E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.55E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.91E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.90E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.80E+01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.80E+01
B	*B* value was obtained from U.S. EPA (1992b).	2.30E+01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	4.36E+04

TABLE A-1-98

CHEMICAL-SPECIFIC INPUTS FOR DIELDRIN (60-57-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.00E-05
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.60E+01
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.75E-04
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.6E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	5.6E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1-99

CHEMICAL-SPECIFIC INPUTS FOR DIETHYL PHTHALATE (84-66-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	222.24
T_m (K)	Montgomery and Welkom (1991)	232.6
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.17E-06 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	8.80E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.48E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.56E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.35E-06
Log K_{ow} (unitless)	Ellington (1996).	2.42
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	8.20E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.20E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.15E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.00E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.00E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.80E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.20E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	4.07E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-99

CHEMICAL-SPECIFIC INPUTS FOR DIETHYL PHTHALATE (84-66-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	8.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1996c)	2.2E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-100

CHEMICAL-SPECIFIC INPUTS FOR DIETHYLSTILBESTROL (56-53-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	268.34
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	443.65
Vp (atm)	U.S. EPA (1995g)	1.40E-12
S (mg/L)	*S* value cited in U.S. EPA (1995b).	1.30E+04
H (atm·m^3/mol)	U.S. EPA (1995g)	3.00E-14
D_a (cm^2/s)	U.S. EPA (1995g)	8.00E-02
D_w (cm^2/s)	U.S. EPA (1995g)	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	5.07
K_{oc} (mL/g)	U.S. EPA (1995g)	9.60E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.60E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.20E+03
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.70E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.80E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.80E+01
B	*B* value was obtained from U.S. EPA (1992b).	1.20E+01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	6.80E+03

TABLE A-1-100

CHEMICAL-SPECIFIC INPUTS FOR DIETHYLSTILBESTROL (56-53-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1996d)	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	4.70E+03
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	4.70E+03
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-101

CHEMICAL-SPECIFIC INPUTS FOR DIMETHOATE (60-51-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	110.98
T_m (K)	--	
Vp (atm)	U.S. EPA (1995g)	4.00E-02
S (mg/L)	U.S. EPA (1995g)	2.80E+03
H (atm·m^3/mol)	U.S. EPA (1995g)	1.25E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.85E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-05
Log K_{ow} (unitless)	Hansch (1995).	0.78
K_{oc} (mL/g)	U.S. EPA (1995g)	9.30E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.30E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.97E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.20E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.00E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.31E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-101

CHEMICAL-SPECIFIC INPUTS FOR DIMETHOATE (60-51-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.0E-04
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1995f)	2.40E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-102

CHEMICAL-SPECIFIC INPUTS FOR 7,12-DIMETHYLBENZ(A)ANTHRACENE (57-97-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	256.35
T_m (K)	--	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.80E-12
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.00E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.11E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.61E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.98E-06
Log K_{ow} (unitless)	Hansch (1995).	5.5
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.55E+05
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.55E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.91E+04
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.60E+00
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	4.20E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAF*s were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	6.31E+04

TABLE A-1-102

CHEMICAL-SPECIFIC INPUTS FOR 7,12-DIMETHYLBENZ(A)ANTHRACENE (57-97-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	2.50E+01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-103

CHEMICAL-SPECIFIC INPUTS FOR 3-3'-DIMETHYLBENZIDINE (119-93-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	212.28
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.90E-10
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.20E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.29E-11
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.83E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.17E-06
Log K_{ow} (unitless)	Hansch (1995).	2.34
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.00E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.00E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.50E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	7.70E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.70E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.10E+00
B	*B* value was obtained from U.S. EPA (1992b).	4.80E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.54E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-103

CHEMICAL-SPECIFIC INPUTS FOR 3-3'-DIMETHYLBENZIDINE (119-93-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2008)	1.1E+01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	1.1E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-104

CHEMICAL-SPECIFIC INPUTS FOR DIMETHYL PHTHALATE (131-11-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	194.19
T_m (K)	Montgomery and Welkom (1991)	273.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.17E-06 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.19E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.01E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.96E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.13E-06
Log K_{ow} (unitless)	Ellington (1996).	1.6
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.74E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.74E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.81E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.60E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.30E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.20E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.70E-03

TABLE A-1-104

CHEMICAL-SPECIFIC INPUTS FOR DIMETHYL PHTHALATE (131-11-3)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	9.68E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	1.00E+01
Oral CSF $(mg/kg/day)^{-1}$	--	NA
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	NA
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	3.30E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-105

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DIMETHYLPHENOL (105-67-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Moses (1978)	122.17
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	300.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	1.66E-04 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	6.25E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.27E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.84E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.69E-06
Log K_{ow} (unitless)	Hansch (1995).	2.3
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1-5 / 126.0 6 / 125.99 7 / 125.9 8 / 125.02 9 / 116.87 10 / 71.06 11 / 15.77 12 / 3.43 13 / 2.05 14 / 1.91
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.26E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.44E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.60E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.20E+00
B	*B* value was obtained from U.S. EPA (1992b).	2.30E-02

TABLE A-1-105

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DIMETHYLPHENOL (105-67-9)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.30E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.00E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	2.12E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-106

CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DIMETHYOXYBENZIDINE (119-90-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	244.28
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	410.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	3.30E-10 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	2.40E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.36E-10
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	2.38E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	5.60E-06
Log K_{ow} (unitless)	Debnath (1992).	1.81
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.02E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.02E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.51E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.20E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.70E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	6.50E+00
B	*B* value was obtained from U.S. EPA (1992b).	6.50E-03

TABLE A-1-106

CHEMICAL-SPECIFIC INPUTS FOR 3,3'-DIMETHYOXYBENZIDINE (119-90-4)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.40E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	1.40E-02
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-107

CHEMICAL-SPECIFIC INPUTS FOR DI-N-BUTYL PHTHALATE (84-74-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	278.34
T_m (K)	Montgomery and Welkom (1991)	238.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.55E-08 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.08E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.43E-06
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	4.38E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	7.86E-06
Log K_{ow} (unitless)	Ellington (1996).	4.5
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.57E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.57E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.18E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	7.20E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.40E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.20E+01
B	*B* value was obtained from U.S. EPA (1992b).	4.10E+00
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s	2.74E+03

TABLE A-1-107

CHEMICAL-SPECIFIC INPUTS FOR DI-N-BUTYL PHTHALATE (84-74-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1996c)	3.0E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-108

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DINITROBENZENE (99-65-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	168.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	363
Vp (atm)	Geometric mean value cited in U.S. EPA (1994f).	4.0E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994f).	5.4E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	1.25E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	3.18E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	9.15E-06
Log K_{ow} (unitless)	Hansch (1995).	1.49
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.92E+01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.92E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.19E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.10E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	9.30E-01
*t** (hr/event)	t* value was obtained from U.S. EPA (1992b).	2.20E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.20E-03

TABLE A-1-108

CHEMICAL-SPECIFIC INPUTS FOR 1,3-DINITROBENZENE (99-65-0)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)	7.40E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.00E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-109

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITRO-6-METHYLPHENOL (534-52-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	198.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	360.65
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.26E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.93E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.91E-06
Log K_{ow} (unitless)	Hansch (1995).	2.13
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.78E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.41E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.39E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.32E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-109

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITRO-6-METHYLPHENOL (534-52-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004c)	1.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	3.5E-04
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-110

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROPHENOL (51-28-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	184.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	385.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.52E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	5.8E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.82E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.73E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.06E-06
Log K_{ow} (unitless)	Hansch (1995).	1.67
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c).	pH / K_{oc} 1 / 0.80 2 / 0.79 3 / 0.72 4 / 0.38 5 / 0.08 6 / 0.02 7-14 / 0.01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	1.0E-04 (at pH 7.0)
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.50E+04 (at pH 7.0)
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.80E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.80E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.50E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.09E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-110

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROPHENOL (51-28-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.0E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	6.2E+00

Note: NA = Not applicable, ND = No data available

TABLE A-1-111

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROTOLUENE (121-14-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Howard (1989-1993)	182.14
T_m (K)	Howard (1989-1993)	344
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.29E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.85E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	1.46E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	3.09E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	7.86E-06
Log K_{ow} (unitless)	Hansch (1995).	1.98
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.84E+01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.84E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.63E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	3.90E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.10E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.70E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.00E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)	5.92E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-111

CHEMICAL-SPECIFIC INPUTS FOR 2,4-DINITROTOLUENE (121-14-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.0E-03
Oral CSF $(mg/kg/day)^{-1}$	The *Oral CSF* value represents a 2,4/2,6-Dinitrotoluene mixture (U.S. EPA 2004b).	6.8E-01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	3.10E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-112

CHEMICAL-SPECIFIC INPUTS FOR 2,6-DINITROTOLUENE (606-20-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Howard (1989-1993)	182.15
T_m (K)	Howard (1989-1993)	339
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	7.47E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.05E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	1.30E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	3.11E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	7.76E-06
Log K_{ow} (unitless)	Nakagawa (1992).	2.1
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.16E+02
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.16E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.70E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	3.10E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.10E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.70E+00
B	*B* value was obtained from U.S. EPA (1992b).	7.40E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)	5.92E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-112

CHEMICAL-SPECIFIC INPUTS FOR 2,6-DINITROTOLUENE (606-20-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S EPA (2008)	1.0E-03
Oral CSF $(mg/kg/day)^{-1}$	The *Oral CSF* value represents a 2,4/2,6-Dinitrotoluene mixture (U.S. EPA 2004b).	6.8E-01
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	3.5E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	--	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	3.1E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-113

CHEMICAL-SPECIFIC INPUTS FOR DI-N-OCTYL PHTHALATE (117-84-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	390.56
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	248.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.90E-09 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.00E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.68E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.32E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.20E-06
Log K_{ow} (unitless)	Ellington (1996).	8.1
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.17E+07
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.17E+05
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.88E+06
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	4.20E+00
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.10E+01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	9.90E+01
B	*B* value was obtained from U.S. EPA (1992b).	1.10E+04

TABLE A-1-113

CHEMICAL-SPECIFIC INPUTS FOR DI-N-OCTYL PHTHALATE (117-84-0)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	3.88E+03
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004c)	4.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.40E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Suter (1996)	1.99E+03

Note: NA = Not applicable, ND = No data available

TABLE A-1-114

CHEMICAL-SPECIFIC INPUTS FOR 1,4-DIOXANE (123-91-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	88.10
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	284.9
Vp (atm)	*Vp* value cited in U.S. EPA (1995g)	5.00E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g)	9.00E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.89E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.20E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.05E-05
Log K_{ow} (unitless)	Hansch (1995).	-0.27
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.32E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.32E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.49E-02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.90E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.00E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.20E-01
B	*B* value was obtained from U.S. EPA (1992b).	4.10E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.67E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-114

CHEMICAL-SPECIFIC INPUTS FOR 1,4-DIOXANE (123-91-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.1E-02
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	1.1E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-115

CHEMICAL-SPECIFIC INPUTS FOR DIPHENYLAMINE (122-39-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	169.23
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.60E-06
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.00E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.96E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.31E-06
Log K_{ow} (unitless)	Hansch (1995).	3.5
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.76E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.76E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.07E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	5.20E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	9.40E-01
*t**	t* value was obtained from U.S. EPA (1992b).	5.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.00E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.69E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-115

CHEMICAL-SPECIFIC INPUTS FOR DIPHENYLAMINE (122-39-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.50E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	8.75E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-116

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIPHENYLHYDRAZINE (122-66-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	184.24
T_m (K)	Montgomery and Welkom (1991)	401.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995g)	4.74E-08 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995g)	6.80E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.28E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.95E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.24E-06
Log K_{ow} (unitless)	Hansch (1995).	2.94
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.77E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.77E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.83E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.01E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-116

CHEMICAL-SPECIFIC INPUTS FOR 1,2-DIPHENYLHYDRAZINE (122-66-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	8.0E-01
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	8.0E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	2.7E+00

Note: NA = Not applicable, ND = No data available

TABLE A-1-117

CHEMICAL-SPECIFIC INPUTS FOR DISULFOTON (298-04-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	274.38
T_m (K)	T_m value cited in U.S. EPA (1995g).	248
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	3.7E-07 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.6E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.12E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.50E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	5.21E-06
Log K_{ow} (unitless)	Hansch (1995).	4.02
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	8.95E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.95E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.71E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.70E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.10E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.40E+01
B	*B* value was obtained from U.S. EPA (1992b).	9.50E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, $_{\text{FW tissue}}$)	--	NA
BAF_{fish} (L/kg FW)	*BAF*s were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	8.79E+02

TABLE A-1-117

CHEMICAL-SPECIFIC INPUTS FOR DISULFOTON (298-04-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	4.00E-05
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-118

CHEMICAL-SPECIFIC INPUTS FOR ENDOSULFAN I (115-29-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	406.95
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	343.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	1.72E-11 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	2.31E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.04E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.59E-03
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.76E-06
Log K_{ow} (unitless)	Hansch (1995).	3.83
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.04E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.04E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.53E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.10E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.70E+01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.90E+02
B	*B* value was obtained from U.S. EPA (1992b).	1.30E+00
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	4.80E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-118

CHEMICAL-SPECIFIC INPUTS FOR ENDOSULFAN I (115-29-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	6.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	5.6E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1-119

CHEMICAL-SPECIFIC INPUTS FOR ENDRIN (72-20-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	380.93
T_m (K)	U.S. EPA (1992a)	473.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a)	7.68E-10 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a)	2.46E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.19E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.07E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	5.76E-06
Log K_{ow} (unitless)	DeBruijn (1989).	5.2
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.08E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.08E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.10E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	3.50E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.80E+01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.90E+01
B	*B* value was obtained from U.S. EPA (1992b).	1.10E+01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	2.01E+03

TABLE A-1-119

CHEMICAL-SPECIFIC INPUTS FOR ENDRIN (72-20-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.00E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	2E-03
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	3.6E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1-120

CHEMICAL-SPECIFIC INPUTS FOR EPICHLOROHYDRIN (1-CHLORO-2,3-EPOXYPROPANE) (106-89-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	92.53
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	247.5
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	2.20E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	6.60E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.08E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.13E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-05
Log K_{ow} (unitless)	DeNeer (1988).	0.45
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.72E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.72E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.04E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	7.80E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.20E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.70E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.80E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.29E-00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-120

CHEMICAL-SPECIFIC INPUTS FOR EPICHLOROHYDRIN (1-CHLORO-2,3-EPOXYPROPANE) (106-89-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2008)	6.0E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	9.90E-03
RfC (mg/m^3)	U.S. EPA (2004b)	1.00E-03
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	4.20E-03
MCL	National Primary Drinking Water Regulations.	2.0E+01 TT[7]
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-121

CHEMICAL-SPECIFIC INPUTS FOR 2-ETHOXYETHANOL (110-80-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	90.12
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.00E-03
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.20E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.23E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.47E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.57E-06
Log K_{ow} (unitless)	Hansch (1995).	-0.32
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.68E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.68E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.01E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.60E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.10E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.40E-01
B	*B* value was obtained from U.S. EPA (1992b).	7.90E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.36E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-121

CHEMICAL-SPECIFIC INPUTS FOR 2-ETHOXYETHANOL (110-80-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	4.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	2.00E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-122

CHEMICAL-SPECIFIC INPUTS FOR ETHYL ACETATE (141-78-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	88.1
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.20E-01
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	6.40E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.38E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.32E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.66E-06
Log K_{ow} (unitless)	Hansch (1995).	0.73
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.53E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.53E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.40E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.70E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.00E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.20E-01
B	*B* value was obtained from U.S. EPA (1992b).	4.90E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.11E-00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-122

CHEMICAL-SPECIFIC INPUTS FOR ETHYL ACETATE (141-78-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	9.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-123

CHEMICAL-SPECIFIC INPUTS FOR ETHYL ETHER (60-29-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	74.12
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.10E-01
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	6.10E+04
H (atm·m^3/mol)	U.S. EPA (1995g)	8.70E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.40E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.30E-06
Log K_{ow} (unitless)	Hansch (1989).	0.89
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.07E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.07E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.55E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.60E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.90E-01
B	*B* value was obtained from U.S. EPA (1992b).	6.80E-04
Biotransfer Factors for Animals		
BCF_{fish} (L//kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.80E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-123

CHEMICAL-SPECIFIC INPUTS FOR ETHYL ETHER (60-29-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.00E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-124

CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHACRYLATE (97-63-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	*MW* value cited in U.S. EPA (1995g)	114.14
T_m (K)	--	NA
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	2.30E-02 at 25°C
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.90E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.38E-04
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	8.07E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	9.35E-06
Log K_{ow} (unitless)	Hansch (1995).	1.94
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.12E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.12E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.09E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.20E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.30E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.90E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.76E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-124

CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHACRYLATE (97-63-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	9.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	3.15E-01
Inhalation URF $(\mu g/m^3)^{-1}$	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-125

CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHANESULFONATE (62-50-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	124.15
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	373.0
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	3.50E-04 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	4.90E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.87E-08
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.63E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.84E-06
Log K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	0.049
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.12E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table for a pH of 7.0.	1.12E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.39E-02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	3.60E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	5.00E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.20E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.10E-04

TABLE A-1-125

CHEMICAL-SPECIFIC INPUTS FOR ETHYL METHANESULFONATE (62-50-0)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	6.42E-01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	–	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-126

CHEMICAL-SPECIFIC INPUTS FOR ETHYLBENZENE (100-41-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	106.16
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	178.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.26E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.73E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.73E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.65E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.49E-06
Log K_{ow} (unitless)	Hansch (1995).	3.15
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.04E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.04E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.53E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	7.30E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.30E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.40E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.46E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-126

CHEMICAL-SPECIFIC INPUTS FOR ETHYLBENZENE (100-41-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	1.00E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	7E-01
Aquatic TRV (ug/l)	U.S. EPA (1995f)	4.53E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-127

CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE DIBROMIDE (106-93-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	187.88
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	282.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.00E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	4.20E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.47E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.17E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.19E-05
Log K_{ow} (unitless)	Hansch (1995).	1.96
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.27E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.27E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.20E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.40E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.90E+00
B	*B* value was obtained from U.S. EPA (1992b).	5.60E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.82E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-127

CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE DIBROMIDE (106-93-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004d)	9.0E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004d)	2.0E+00
RfC (mg/m^3)	U.S. EPA (2004d)	9.1E-03
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004d)	2.1E+00
MCL	National Primary Drinking Water Regulations.	5E-05
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-128

CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE THIOUREA (ETU) (96-45-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	102.17
T_m (°K)	Budavari, O'Neill, Smith, and Heckelman (1989)	476.65
Vp	Geometric mean value cited in U.S. EPA (1994c).	1.10E-04
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.20E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.08E-10
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.15E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.02E-05
Log K_{ow} (unitless)	Govers (1986).	-0.66
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.25E-01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.25E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.68E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.50E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.70E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.80E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.20E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.86E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-128

CHEMICAL-SPECIFIC INPUTS FOR ETHYLENE THIOUREA (ETU) (96-45-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	8.0E-05
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	1.10E-01
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	2.8E-04
Inhalation CSF $(mg/kg/day)^{-1}$	Route to route extrapolation from Oral CSF.	1.10E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: ND = Not applicable, ND = No data available

TABLE A-1-129

CHEMICAL-SPECIFIC INPUTS FOR FLUORANTHENE (206-44-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	202.26
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	383.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.07E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.32E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.33E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.75E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.18E-06
Log K_{ow} (unitless)	Hansch (1995).	5.16
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.91E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.91E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.68E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	4.80E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.50E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.20E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.30E+01

TABLE A-1-129

CHEMICAL-SPECIFIC INPUTS FOR FLUORANTHENE (206-44-0)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg $_{FW\ tissue}$)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	2.06E+04
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	4.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.4E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	4.0E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-130

CHEMICAL-SPECIFIC INPUTS FOR FLUORENE (86-73-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	166.22
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	389.1
Vp (atm)	*Vp* value cited in U.S. EPA (1998c).	8.17E-07 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	1.90E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.30E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	3.63E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	7.88E-06
Log K_{ow} (unitless)	Hansch (1995)	4.18
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	7.71E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.71E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.78E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.80E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	9.00E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.40E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.60E+00
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	1.22E+03

TABLE A-1-130

CHEMICAL-SPECIFIC INPUTS FOR FLUORENE (86-73-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	4.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.40E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1996c)	4.0E+00

Note: NA = Not applicable, ND = No data available

TABLE A-1-131

CHEMICAL-SPECIFIC INPUTS FOR FLUORIDE (16984-48-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	--	18.9984
T_m (K)	--	NA
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	D_a was calculated using equations cited and recommended for use in U.S. EPA (1997g).	0.26684
D_w (cm^2/s)	D_w was calculated using equations cited and recommended for use in U.S. EPA (1997g).	3.09E-05
Log K_{ow} (unitless)	U.S. EPA (2000).	2.23E-01
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	--	NA
ô (hr)	--	NA
t (hr/event)*	--	NA
B	--	NA
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-131

CHEMICAL-SPECIFIC INPUTS FOR FLUORIDE (16984-48-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	6.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	NA
RfC (mg/m^3)	--	NA
Inhalation CSF $(mg/kg/day)^{-1}$	--	NA
MCL (mg/L)	National Primary Drinking Water Regulations.	4
Aquatic TRV (µg/l)	--	NA

Note: NA = Not applicable, ND = No data available

TABLE A-1-132

CHEMICAL-SPECIFIC INPUTS FOR FORMALDEHYDE (50-00-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	30.03
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	365.1
Vp (atm)	*Vp* value cited in U.S. EPA (1994c)	5.10E+00 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995g)	5.50E+05
H (atm·m^3/mol)	*H* value value cited in Betteron and Hoffmann (1988)	3.37E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.80E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	1.98E-05
Log K_{ow} (unitless)	Hansch (1995).	0.35
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.27E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.27E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.70E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.20E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.30E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.20E-01
B	*B* value was obtained from U.S. EPA (1992b).	8.90E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)	1.07E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-132

CHEMICAL-SPECIFIC INPUTS FOR FORMALDEHYDE (50-00-0)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	ATSDR (1999)	9.99E-03
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	4.50E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-133

CHEMICAL-SPECIFIC INPUTS FOR FORMIC ACID (64-18-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1995g)	46.03
T_m (K)	U.S. EPA (1995g)	282.0
Vp (atm)	*Vp* value cited in U.S. EPA (1995g)	5.40E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g)	1.00E+06
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.49E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.22E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.71E-05
Log K_{ow} (unitless)	Hansch (1995)	-0.54
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.47E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.47E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.36E-02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	4.10E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.70E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.00E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.90E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.29E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-133

CHEMICAL-SPECIFIC INPUTS FOR FORMIC ACID (64-18-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	2.00E+00
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004c)	3.0E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-134

CHEMICAL-SPECIFIC INPUTS FOR FURAN (110-00-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	68.08
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.90E-01
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.00E+04
H (atm·m^3/mol)	U.S. EPA (1995g)	5.40E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.04E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.22E-05
Log K_{ow} (unitless)	Hansch (1995).	1.34
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.38E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.38E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.03E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	6.50E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.30E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.50E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.20E-03
Biotransfer Factors for Animals		
BCF_{fish} (unitless, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	6.14E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-134

CHEMICAL-SPECIFIC INPUTS FOR FURAN (110-00-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.00-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-135

CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR (76-44-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	373.35
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	368.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	4.29E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.73E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.87E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.12E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.69E-06
Log K_{ow} (unitless)	Simpson (1995).	6.1
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	9.53E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.53E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.15E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.80E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.70E+01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.80E+01
B	*B* value was obtained from U.S. EPA (1992b).	1.80E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg $_{FW\ tissue}$)	*BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)	5.52E+03

TABLE A-1-135

CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR (76-44-8)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a *BCF*. *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998).	1.05E+05

TABLE A-1-135

CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR (76-44-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.00E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	4.50E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	4.55E+00
MCL	National Primary Drinking Water Regulations.	4E-04
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	3.8E-03

Note: NA = Not applicable, ND = No data available

TABLE A-1-136

CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR EPOXIDE (1024-57-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	389.32
T_m (K)	Montgomery and Welkom (1991)	430.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	5.79E-09 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a) .	2.68E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.29E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.32E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.23E-06
Log K_{ow} (unitless)	Sangster (1993).	4.98
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.86E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.86E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.90E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.90E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.10E+01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.00E+02
B	*B* value was obtained from U.S. EPA (1992b).	1.00E+01

TABLE A-1-136

CHEMICAL-SPECIFIC INPUTS FOR HEPTACHLOR EPOXIDE (1024-57-3)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	1.14E+04
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.30E-05
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	9.1E+00
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	4.6E-05
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	9.1E+00
MCL	National Primary Drinking Water Regulations.	2E-04
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	3.8E-03

Note: NA = Not applicable, ND = No data available

TABLE A-1-137

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLORO-1,3-BUTADIENE (PERCHLOROBUTADIENE) (87-68-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	260.76
T_m (K)	Montgomery and Welkom (1991)	252.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.33E-04 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.54E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.39E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.73E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.33E-06
Log K_{ow} (unitless)	Hansch (1995).	4.78
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.00E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.00E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.75E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.30E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.40E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.70E+01
B	*B* value was obtained from U.S. EPA (1992b).	6.50E+00
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	6.20E+03

TABLE A-1-137

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLORO-1,3-BUTADIENE (PERCHLOROBUTADIENE) (87-68-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2007a)	1.0E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	7.80E-02
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	7.80E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	9.3E-01

Note: NA = Not applicable, ND = No data available

TABLE A-1-138

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROBENZENE (118-74-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	284.8
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	504.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.62E-08 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	8.62E-03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	5.35E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database U.S. EPA (1994d).	1.41E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database U.S. EPA (1994d).	7.84E-06
Log K_{ow} (unitless)	DeBruijn (1989).	5.73
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	8.00E+04
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.00E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.00E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.30E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.80E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.30E+01
B	*B* value was obtained from U.S. EPA (1992b).	7.80E+01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	5.52E+04

TABLE A-1-138

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROBENZENE (118-74-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	8.0E-04
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	1.6E+00
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	1.6E+00
MCL	National Primary Drinking Water Regulations.	1E-03
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-139

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOHEXANE, ALPHA (ALPHA-BHC) (319-84-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.85
T_m (K)	Montgomery and Welkom (1991)	385.65
Vp (mmHG)	Geometric mean value cited in U.S. EPA (1994c).	9.40 E-06
S (in water)	U.S. EPA (1995g)	4.20E+00
H (atm·m^3/mol)	U.S. EPA (1995g).	3.40E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.42E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.34E-06
Log K_{ow} (unitless)	Hansch (1995).	3.8
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.60E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.60E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.45E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.40E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	5.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	5.40E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	4.56E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-139

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOHEXANE, ALPHA (ALPHA-BHC) (319-84-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	ATSDR (2005)	8.0E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	6.30E+00
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.75E-03
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	6.30E+00
MCL	National Primary Drinking Water Regulations.	2E-04
Aquatic TRV (µg/l)	U.S. EPA (1995f)	8E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1-140

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOHEXANE, BETA (BETA-BHC) (319-85-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.85
T_m (K)	Montgomery and Welkom (1991)	385.65
Vp (mmHG)	Geometric mean value cited in U.S. EPA (1994c).	9.40 E-06
S (in water)	U.S. EPA (1995g)	4.20E+00
H (atm·m^3/mol)	U.S. EPA (1995g).	3.40E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.42E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.34E-06
Log K_{ow} (unitless)	Hansch (1995).	4.14
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.60E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.60E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.45E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.40E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	5.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	5.40E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	1.14E+03

TABLE A-1-140

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOHEXANE, BETA (BETA-BHC) (319-85-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	ATSDR (2005) (based on the intermediate exposure MRL)	6.00E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.8E+00
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.4E-04
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.8E+00
MCL	National Primary Drinking Water Regulations.	2E-04
Aquatic TRV (µg/l)	U.S. EPA (1995f)	8E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1-141

CHEMICAL-SPECIFIC INPUTS FOR GAMMA-HEXACHLOROCYCLOHEXANE (LINDANE) (58-89-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.85
T_m (K)	Montgomery and Welkom (1991)	385.65
Vp (mmHG)	Geometric mean value cited in U.S. EPA (1994c).	9.40 E-06
S (in water)	U.S. EPA (1995g)	4.20E+00
H (atm·m^3/mol)	U.S. EPA (1995g).	3.40E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.42E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.34E-06
Log K_{ow} (unitless)	Hansch (1995).	3.72
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.60E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.60E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.45E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.40E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	5.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	5.40E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.96E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-141

CHEMICAL-SPECIFIC INPUTS FOR GAMMA-HEXACHLOROCYCLOHEXANE (LINDANE) (58-89-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.00E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.30E+00
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.05E-03
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	1.30E+00
MCL	National Primary Drinking Water Regulations.	2E-04
Aquatic TRV (µg/l)	U.S. EPA (1995f)	8E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1-142

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOPENTADIENE (77-47-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	272.77
T_m (K)	Montgomery and Welkom (1991)	264.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	9.63E-05 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.53E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.72E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.61E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.21E-06
Log K_{ow} (unitless)	Hansch (1995).	5.04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.01E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.01E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.76E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.80E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.00E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.90E+01
B	*B* value was obtained from U.S. EPA (1992b).	2.50E+01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	5.25E+02

TABLE A-1-142

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROCYCLOPENTADIENE (77-47-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	6.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	2.0E-04
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	5E-02
Aquatic TRV (ug/l)	U.S. EPA (1995f)	7.0E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1-143

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROETHANE (67-72-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, Heckelman (1989)	236.74
T_m (K)	Montgomery and Welkom (1991)	459.7
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	6.21E-04 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.08E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.60E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.77E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.88E-06
Log K_{ow} (unitless)	Hansch (1995).	4.14
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.27E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.27E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.71E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	4.70E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.40E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.00E+01
B	*B* value was obtained from U.S. EPA (1992b).	1.00E+00
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)	6.29E+02

TABLE A-1-143

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROETHANE (67-72-1)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	*BAF*s were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	8.68E+02

TABLE A-1-143

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROETHANE (67-72-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.00E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.40E-02
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.40E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	9.8

Note: NA = Not applicable, ND = No data available

TABLE A-1-144

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPHENE (70-30-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith and Heckleman (1989)	406.92
T_m (K)	Budavari, O'Neil, Smith and Heckleman (1989)	437.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	3.60E-15 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	3.0E-03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.88E-10
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	3.46E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	4.01E-06
Log K_{ow} (unitless)	Hansch (1995).	7.54
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.12E+06
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.12E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.40E+04
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.40E+00
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.70E+01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.30E+02
B	*B* value was obtained from U.S. EPA (1992b).	3.50E+03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	4.66E+03

TABLE A-1-144

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPHENE (70-30-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.00E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-145

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPROPENE (1888-71-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	248.75
T_m (K)	CRC Handbook (1995)	200.25
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from WATER8 model database (U.S. EPA 1995d).	4.70E-03
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	8.00E-06
Log K_{ow} (unitless)	U.S. EPA (2000).	4.376
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.88E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-145

CHEMICAL-SPECIFIC INPUTS FOR HEXACHLOROPROPENE (1888-71-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-146

CHEMICAL-SPECIFIC INPUTS FOR HEXAHYDRO-1,3,5-TRINITRO-1,3,5-TRIAZINE (121-82-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.85
T_m (K)	Montgomery and Welkom (1991)	385.65
Vp (mmHG)	Geometric mean value cited in U.S. EPA (1994c).	9.40 E-06
S (in water)	U.S. EPA (1995g)	4.20E+00
H (atm·m^3/mol)	U.S. EPA (1995g).	3.40E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.42E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.34E-06
Log K_{ow} (unitless)	Sangster (1993).	0.87
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.60E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.60E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.45E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.40E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	5.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	5.40E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.70E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-146

CHEMICAL-SPECIFIC INPUTS FOR HEXAHYDRO-1,3,5-TRINITRO-1,3,5-TRIAZINE (121-82-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.00E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.1E-01
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.05E-02
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on Oral CSF assuming route-to-route extrapolation.	1.1E-01
MCL	National Primary Drinking Water Regulations.	2E-04
Aquatic TRV (µg/l)	U.S. EPA (1995f)	8E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1-147

CHEMICAL-SPECIFIC INPUTS FOR INDENO(1,2,3-CD)PYRENE (193-39-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	276.34
T_m (K)	Montgomery and Welkom (1991)	435
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.88E-13 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.07E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	4.86E-09
D_a (cm^2/s)	D_a value was obtained from WATER8 model database U.S. EPA (1995d)	1.90E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database U.S. EPA (1995d)	5.66E-06
Log K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	6.91
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.21E+06
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.21E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.65E+05
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.10E+00
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.00E+01
B	*B* value was obtained from U.S. EPA (1992b).	4.50E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	1.31E+04

TABLE A-1-147

CHEMICAL-SPECIFIC INPUTS FOR INDENO(1,2,3-CD)PYRENE (193-39-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	Calculated by multiplying the *Oral CSF* for Benzo(a)pyrene by the relative potency factor for Indeno(1,2,3-cd)pyrene of 0.1 (U.S. EPA 1993b).	7.3E-01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1993b) and Thyssen (1981)	3.10E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-148

CHEMICAL-SPECIFIC INPUTS FOR IRON (7439-89-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	55.84
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	1808.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	--	NA
D_w (cm^2/s)	--	NA
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.00E-03
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-148

CHEMICAL-SPECIFIC INPUTS FOR IRON (7439-89-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--.	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	1.0E+03

Note: NA = Not applicable, ND = No data available

TABLE A-1-149

CHEMICAL-SPECIFIC INPUTS FOR ISOBUTYL ALCOHOL (78-83-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	74.14
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.40E-02
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.60E+04
H (atm·m^3/mol)	U.S. EPA (1995g)	1.30E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.60E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.30E-06
Log K_{ow} (unitless)	Hansch (1995).	0.76
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.79E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.79E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.59E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.30E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.90E-01
B	*B* value was obtained from U.S. EPA (1992b).	5.60E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.23E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-149

CHEMICAL-SPECIFIC INPUTS FOR ISOBUTYL ALCOHOL (78-83-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.05E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-150

CHEMICAL-SPECIFIC INPUTS FOR ISOPHORONE (78-59-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	138.21
T_m (K)	Montgomery and Welkom (1991)	265.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	5.38E-04 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.20E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.20E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.22E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.50E-06
Log K_{ow} (unitless)	Veith (1980).	1.7
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.69E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.69E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.52E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	4.40E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	6.10E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.50E+00
B	*B* value was obtained from U.S. EPA (1992b).	5.00E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.15E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-150

CHEMICAL-SPECIFIC INPUTS FOR ISOPHORONE (78-59-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.00E-01
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.0E-03
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.00E-01
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	9.50E-04
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.170E+03

Note: NA = Not applicable, ND = No data available

TABLE A-1-151

CHEMICAL-SPECIFIC INPUTS FOR KEPONE (143-50-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	490.68
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.90E-10
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.60E+00
H (atm·m^3/mol)	U.S. EPA (1995g)	2.55E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	5.41
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.08E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.08E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.56E+04
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	8.60E+01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.10E+02
B	*B* value was obtained from U.S. EPA (1992b).	2.00E+01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAF*s were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	5.39E+04

TABLE A-1-151

CHEMICAL-SPECIFIC INPUTS FOR KEPONE (143-50-0)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004c)	2.0E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004c)	8.0E+00
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.0E-04
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	8.0E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-152

CHEMICAL-SPECIFIC INPUTS FOR LEAD (7439-92-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	207.2
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	600.5
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	5.43E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	6.28E-06
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from Baes, Sharp, Sjoreen, and Shor (1984), which states that several factors, such as experimental methods and soil type, could influence partitioning or Kd_s values. Baes, Sharp, Sjoreen, and Shor (1984) compares values between various literature sources and provide this value, which is based on its best judgment.	9.00E+02
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e).	9.00E+02
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (day/kg FW)	Because lead is hydrophobic, *BAF* was used. BAF_{fish} value was obtained from NC DEHNR (1997).	8.0

TABLE A-1-152

CHEMICAL-SPECIFIC INPUTS FOR LEAD (7439-92-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	Action level=1.5E-02; TT[6]
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	2.5E+00

Note: NA = Not applicable, ND = No data available

TABLE A-1-153

CHEMICAL-SPECIFIC INPUTS FOR MAGNESIUM (7439-95-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	24.30
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	924.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	--	NA
D_w (cm^2/s)	--	NA
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-153

CHEMICAL-SPECIFIC INPUTS FOR MAGNESIUM (7439-95-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-154

CHEMICAL-SPECIFIC INPUTS FOR MALATHION (121-75-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.85
T_m (K)	Montgomery and Welkom (1991)	385.65
Vp (mmHG)	Geometric mean value cited in U.S. EPA (1994c).	9.40 E-06
S (in water)	U.S. EPA (1995g)	4.20E+00
H (atm·m^3/mol)	U.S. EPA (1995g).	3.40E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.42E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.34E-06
Log K_{ow} (unitless)	Hansch (1995).	2.36
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.60E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.60E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.45E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.40E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	5.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	5.40E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.66E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-154

CHEMICAL-SPECIFIC INPUTS FOR MALATHION (121-75-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.0E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	2E-04
Aquatic TRV (µg/l)	U.S. EPA (1995f)	8E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1-155

CHEMICAL-SPECIFIC INPUTS FOR MANGANESE (7439-96-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	54.94
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1517.15
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	8.00E-06
Log K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-155

CHEMICAL-SPECIFIC INPUTS FOR MANGANESE (7439-96-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.40E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	5.00E-05
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1996c)	8.00E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-156

CHEMICAL-SPECIFIC INPUTS FOR MERCURY (7439-97-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	200.59
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	234.23
Vp (atm)	Budavari, O'Neil, Smith, and Heckelman (1989)	2.63E-06 at 25°C
S (mg/L)	Budavari, O'Neil, Smith, and Heckelman (1989)	5.62E-02
H (atm·m^3/mol)	U.S. EPA (1997g)	7.1E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database in U.S. EPA (1994d). CHEMDAT8 uses correlations with density and molecular weight to calculate D_a values. A density value of 13.546 g/cc for mercury was used.	1.09E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database in U.S. EPA (1994d). CHEMDAT8 uses correlations with density and molecular weight to calculate D_w values. A density value of 13.546 g/cc for mercury was used.	3.01E-05
Log K_{ow} (unitless)	Daylight (1999).	0.62
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	U.S. EPA (1997g)	1.00E+03
Kd_{sw} (L/Kg)	U.S. EPA (1997g)	3.00E+03
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/g FW tissue)	--	NA
BAF_{fish} (L/kg FW)	Elemental mercury does not deposit onto soils and surface water. Therefore, there is no transfer of elemental mercury into the fish tissue.	NA

TABLE A-1-156

CHEMICAL-SPECIFIC INPUTS FOR MERCURY (7439-97-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	3.0E-04
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	2E-03
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	7.7E-01

Note: NA = Not available, ND = No data available

TABLE A-1-157

CHEMICAL-SPECIFIC INPUTS FOR METHACRYLONITRILE (126-98-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	67.09
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	237.3
Vp (atm)	*Vp* value cited in U.S. EPA (1995g)	8.90E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g)	2.50E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.39E-04
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.15E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.33E-05
Log K_{ow} (unitless)	Tanii (1984).	0.68
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.14E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.14E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.10E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.80E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.20E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.40E-01
B	*B* value was obtained from U.S. EPA (1992b).	3.50E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.94E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-157

CHEMICAL-SPECIFIC INPUTS FOR METHACRYLONITRILE (126-98-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	7.0E-04
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-158

CHEMICAL-SPECIFIC INPUTS FOR METHANOL (67-56-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	32.04
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	175.3
Vp (atm)	*Vp* value cited in Montgomery and Welkom (1991)	1.30E-01 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g)	2.90E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.44E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	4.58E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.64E-05
Log K_{ow} (unitless)	Hansch (1995).	-0.77
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.94E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.94E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.21E-02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	3.80E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.40E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.30E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.90E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.53E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-158

CHEMICAL-SPECIFIC INPUTS FOR METHANOL (67-56-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-159

CHEMICAL-SPECIFIC INPUTS FOR METHOXYCHLOR (72-43-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	345.65
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	351.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.62E-09 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	8.84E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.33E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.30E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.59E-06
Log K_{ow} (unitless)	Hansch (1995).	5.08
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	8.00E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	8.00E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.00E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	6.00E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.10E+01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.40E+01
B	*B* value was obtained from U.S. EPA (1992b).	1.20E+01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	1.56E+04

TABLE A-1-159

CHEMICAL-SPECIFIC INPUTS FOR METHOXYCHLOR (72-43-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.75E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	4E-02
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	3.0E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1-160

CHEMICAL-SPECIFIC INPUTS FOR METHYL ACETATE (79-20-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	290.85
T_m (K)	Montgomery and Welkom (1991)	385.65
Vp (mmHG)	Geometric mean value cited in U.S. EPA (1994c).	9.40 E-06
S (in water)	U.S. EPA (1995g)	4.20E+00
H (atm·m^3/mol)	U.S. EPA (1995g).	3.40E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.42E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.34E-06
Log K_{ow} (unitless)	Hansch (1995).	0.18
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	4.60E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.60E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.45E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.40E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	5.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	5.40E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	8.07E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-160

CHEMICAL-SPECIFIC INPUTS FOR METHYL ACETATE (79-20-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	1.0E+00
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	2E-04
Aquatic TRV (µg/l)	U.S. EPA (1995f)	8E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1-161

CHEMICAL-SPECIFIC INPUTS FOR METHYL BROMIDE (74-83-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith and Heckelman (1989)	94.95
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	179.44
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.16E+00 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.45E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.41E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.28E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.21E-05
Log K_{ow} (unitless)	Hansch (1995).	1.19
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	9.00E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.00E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.75E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	3.50E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.30E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.00E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.50E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	4.72E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-161

CHEMICAL-SPECIFIC INPUTS FOR METHYL BROMIDE (74-83-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.40E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	5.00E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.10E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-162

CHEMICAL-SPECIFIC INPUTS FOR METHYL CHLORIDE (74-87-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	50.49
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	176.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.68E+00 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	6.34E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.52E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.13E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.39E-05
Log K_{ow} (unitless)	Hansch (1995).	0.91
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	6.00E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.00E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.50E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	4.20E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.80E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.30E-01
B	*B* value was obtained from U.S. EPA (1992b).	8.10E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.89E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-162

CHEMICAL-SPECIFIC INPUTS FOR METHYL CHLORIDE (74-87-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (1997d)	9.1E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	5.5E+03

Note: NA = Not applicable, ND = No data available

TABLE A-1-163

CHEMICAL-SPECIFIC INPUTS FOR METHYL ETHYL KETONE (78-93-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	72.10
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	187.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.20E-01 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	2.40E+05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.61E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.35E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.03E-05
Log K_{ow} (unitless)	Hansch (1995).	0.29
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.03E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.03E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.52E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.10E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.40E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.80E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.90E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	9.78E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-163

CHEMICAL-SPECIFIC INPUTS FOR METHYL ETHYL KETONE (78-93-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	6.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	4.9E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-164

CHEMICAL-SPECIFIC INPUTS FOR METHYL ISOBUTYL KETONE (108-10-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	100.16
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	188.4
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	2.50E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	2.00E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.25E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.59E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.36E-06
Log K_{ow} (unitless)	Tanii (1986).	1.31
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.31E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.31E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.79E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	3.30E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.60E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.60E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.50E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	5.83E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-164

CHEMICAL-SPECIFIC INPUTS FOR METHYL ISOBUTYL KETONE (108-10-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	8.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	3.01E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-165

CHEMICAL-SPECIFIC INPUTS FOR METHYL MERCURY (22967-92-6) (FISH PATHWAY ONLY)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1997g)	216.0
T_m (°K)	--	ND
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	U.S. EPA (1997g)	4.7E-07
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1997g).	5.28E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	6.11E-06
Log K_{ow} (unitless)	U.S. EPA (2000).	0.08
K_{oc} (mL/g)	--	ND
Kd_s (mL/g)	U.S. EPA (1997g)	7.00E+03
Kd_{sw} (L/Kg)	U.S. EPA (1997g)	1.00E+05
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	Defaulô value cited in U.S. EPA (1997g) for a Trophic Level 4 fish (6.80E+06), multiplied by 15% to adjust for the maximum fraction of total mercury assumed to by methylated in surface water .	1.02E+06

TABLE A-1-165

CHEMICAL-SPECIFIC INPUTS FOR METHYL MERCURY (22967-92-6) (FISH PATHWAY ONLY)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not Applicable, ND = No data available

TABLE A-1-166

CHEMICAL-SPECIFIC INPUTS FOR METHYL METHACRYLATE (80-62-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	100.13
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	5.10E-02
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.60E+04
H (atm·m^3/mol)	U.S. EPA (1995g)	3.20E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.70E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.60E-06
Log K_{ow} (unitless)	Hansch (1995).	1.38
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.48E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.48E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.11E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.50E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.60E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.60E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.40E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	6.59E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-166

CHEMICAL-SPECIFIC INPUTS FOR METHYL METHACRYLATE (80-62-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.4E+00
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	7.0E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-167

CHEMICAL-SPECIFIC INPUTS FOR METHYL-5-NITROANILINE, 2- (5-NITRO-O-TOLUIDINE) (99-55-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	268.34
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	452.65
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.4E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.09E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.36E-06
Log K_{ow} (unitless)	Hansch (1995).	1.87
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.60E+00
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.80E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.80E+01
B	*B* value was obtained from U.S. EPA (1992b).	2.60E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980).	1.55E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-167

CHEMICAL-SPECIFIC INPUTS FOR METHYL-5-NITROANILINE, 2- (5-NITRO-O-TOLUIDINE) (99-55-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	3.3E-02
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	3.3E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-168

CHEMICAL-SPECIFIC INPUTS FOR METHYL PARATHION (298-00-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	263.23
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	310.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	1.30E-08 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	5.00E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.84E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.87E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.43E-06
Log K_{ow} (unitless)	Hansch (1995).	2.86
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.48E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.48E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.86E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.40E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.50E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.50E+00
B	*B* value was obtained from U.S. EPA (1992b).	7.90E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	8.78E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-168

CHEMICAL-SPECIFIC INPUTS FOR METHYL PARATHION (298-00-0)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.54E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	8.75E-04
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-169

CHEMICAL-SPECIFIC INPUTS FOR 3-METHYLCHOLANTHRENE (56-49-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	268.34
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	452.65
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.4E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.09E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.36E-06
Log K_{ow} (unitless)	Hansch (1995).	6.42
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.05E+06
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.05E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.54E+05
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.60E+00
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.80E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.80E+01
B	*B* value was obtained from U.S. EPA (1992b).	2.60E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg $_{FW\ tissue}$)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and	1.10E+06

TABLE A-1-169

CHEMICAL-SPECIFIC INPUTS FOR 3-METHYLCHOLANTHRENE (56-49-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	CalEPA (1992)	2.2E+01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	2.2E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-170

CHEMICAL-SPECIFIC INPUTS FOR METHYLENE BROMIDE (74-95-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	263.23
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	310.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	1.30E-08 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	5.00E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.84E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.87E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.43E-06
Log K_{ow} (unitless)	Martiska (1990).	1.7
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.66E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.66E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.99E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.40E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.50E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.50E+00
B	*B* value was obtained from U.S. EPA (1992b).	7.90E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.15E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-170

CHEMICAL-SPECIFIC INPUTS FOR METHYLENE BROMIDE (74-95-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	1.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	3.5E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-171

CHEMICAL-SPECIFIC INPUTS FOR METHYLENE CHLORIDE (75-09-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	84.93
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	310.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	1.30E-08 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	5.00E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.84E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.87E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.43E-06
Log K_{ow} (unitless)	Hansch (1995).	1.25
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.17E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.17E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.78E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.40E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.50E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.50E+00
B	*B* value was obtained from U.S. EPA (1992b).	7.90E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	5.25E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-171

CHEMICAL-SPECIFIC INPUTS FOR METHYLENE CHLORIDE (75-09-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	6.0E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	7.5E-03
RfC (mg/m^3)	ATSDR (2000)	1.06E+00
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.65E-03
MCL	National Primary Drinking Water Regulations.	5.0E-03
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-172

CHEMICAL-SPECIFIC INPUTS FOR 2-METHYLNAPTHALENE (91-57-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	142.20
T_m (K)	CRC Handbook (1995)	307.55
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.05E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.84E-06
Log K_{ow} (unitless)	Hansch (1995).	3.86
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.42E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	6.44E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.87E+00
B	*B* value was obtained from U.S. EPA (1992b).	7.24E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-172

CHEMICAL-SPECIFIC INPUTS FOR 2-METHYLNAPTHALENE (91-57-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	4.0E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-173

CHEMICAL-SPECIFIC INPUTS FOR MOLYBDENUM (7439-98-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	95.94
T_m (K)	--	N/A
Vp (atm)	--	N/A
S (mg/L)	--	N/A
H (atm·m^3/mol)	--	N/A
D_a (cm^2/s)	--	N/A
D_w (cm^2/s)	--	N/A
Log K_{ow} (unitless)	--	N/A
K_{oc} (mL/g)	--	N/A
Kd_s (cm^3/g)	U.S. EPA (1995g)	2.00E+01
Kd_{sw} (L/Kg)	--	2.00E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	ND
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-173

CHEMICAL-SPECIFIC INPUTS FOR MOLYBDENUM (7439-98-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1996c)	2.40E+00

Note: NA = Not applicable, ND = No data available

TABLE A-1-174

CHEMICAL-SPECIFIC INPUTS FOR NAPHTHALENE (91-20-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	128.16
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	353.3
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.17E-04 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.11E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.82E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	5.26E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d)	8.92E-06
Log K_{ow} (unitless)	Hansch (1995)..	3.3
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.19E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.19E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.92E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	7.70E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	5.30E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.40E+00
B	*B* value was obtained from U.S. EPA (1992b).	2.30E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.90E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-174

CHEMICAL-SPECIFIC INPUTS FOR NAPHTHALENE (91-20-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	3.0E-03
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004e) (provisional value) and U.S. EPA (2006).	3.5E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	6.2E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-175

CHEMICAL-SPECIFIC INPUTS FOR 1,4-NAPHTHAQUINONE (130-15-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	158.15
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	399.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.60E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.98E-06
Log K_{ow} (unitless)	Hansch (1995).	1.71
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.39E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	8.05E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.93E+00
B	*B* value was obtained from U.S. EPA (1992b).	5.13E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-175

CHEMICAL-SPECIFIC INPUTS FOR 1,4-NAPHTHAQUINONE (130-15-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-176

CHEMICAL-SPECIFIC INPUTS FOR 2-NAPHTHYLAMINE (91-59-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	143.18
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	323.15
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	U.S. EPA (1995g)	6.03E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.51E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.39E-06
Log K_{ow} (unitless)	Hansch (1995).	2.28
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.74E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.74E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.31E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	6.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.60E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.90E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.18E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-176

CHEMICAL-SPECIFIC INPUTS FOR 2-NAPHTHYLAMINE (91-59-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-177

CHEMICAL-SPECIFIC INPUTS FOR NICKEL (7440-02-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	58.69
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1,828
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.26E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.46E-05
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. The default value used by DRAS is based on the most neutral pH (6.8).	16 at pH=4.9; 65 at pH=6.8; 1,900 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). The default value used by DRAS is based on the most neutral pH (6.8).	16 at pH=4.9; 65 at pH=6.8; 1,900 at pH=8.0
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b)	7.80E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-177

CHEMICAL-SPECIFIC INPUTS FOR NICKEL (7440-02-0)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	8.4E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	5.2E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-178

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROANILINE (88-74-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	138.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	342.1
Vp (atm)	*Vp* value cited in Montgomery and Welcom (1991).	1.07E-05 at 25°C (solid)
S (mg/L)	*S* value cited in Montgomery and Welcom (1991).	1.26E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.17E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.29E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.81E-06
Log K_{ow} (unitless)	Hansch (1995).	1.85
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.59E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.59E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.94E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.50E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-178

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROANILINE (88-74-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.0E-03
Oral CSF $(mg/kg/day)^{-1}$	--	NA
RfC (mg/m^3)	U.S. EPA (2004c)	1.05E-04
Inhalation CSF $(mg/kg/day)^{-1}$	--	NA
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-179

CHEMICAL-SPECIFIC INPUTS FOR 3-NITROANILINE (99-09-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	138.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	387.1
Vp (atm)	--	1.07E-05 at 25°C (solid)
S (mg/L)	*S* value cited in Montgomery and Welcom (1991)	8.90E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant.	1.65E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	7.11E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.23E-06
Log K_{ow} (unitless)	Hansch (1995).	1.37
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.22E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.22E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.67E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.57E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	6.09E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.46E+00
B	*B* value was obtained from U.S. EPA (1992b).	2.34E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)	5.92E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-179

CHEMICAL-SPECIFIC INPUTS FOR 3-NITROANILINE (99-09-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004c)	3.0E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004c)	2.1E-02
RfC (mg/m^3)	U.S. EPA (2004c)	3.0E+00
Inhalation CSF $(mg/kg/day)^{-1}$	Route to route extrapolation from Oral CSF.	2.1E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-180

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROANILINE (100-01-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	138.12
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	419.10
Vp (atm)	--	ND
S (mg/L)	*S* value cited in Montgomery and Welcom (1991)	1.07E-05
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant.	1.65E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.31E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.75E-06
Log K_{ow} (unitless)	Hansch (1995).	1.39
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.33E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.33E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.74E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.33E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	6.09E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.46E+00
B	*B* value was obtained from U.S. EPA (1992b).	2.04E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	6.71E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-180

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROANILINE (100-01-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004c)	3.00E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004c)	2.1E-02
RfC (mg/m^3)	U.S. EPA (2004c)	3.5E-03
Inhalation CSF $(mg/kg/day)^{-1}$	Route to route extrapolation from Oral CSF.	2.1E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-181

CHEMICAL-SPECIFIC INPUTS FOR NITROBENZENE (98-95-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	123.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	279.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	3.21E-04 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.92E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	2.06E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	5.43E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	9.43E-06
Log K_{ow} (unitless)	Hansch (1995).	1.85
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.19E+02
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.19E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.90E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	6.80E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.20E+00
B	*B* value was obtained from U.S. EPA (1992b).	6.90E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). *BCF* values were geometric mean laboratory or field derived values obtained from various literature sources cited in U.S. EPA (1998)	5.92E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-181

CHEMICAL-SPECIFIC INPUTS FOR NITROBENZENE (98-95-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (1997c)	2.0E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	2.70E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-182

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPHENOL (88-75-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	139.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	317.1
Vp (atm)	*Vp* value cited in Howard (1989-1993).	2.63E-04 at 25°C (solid)
S (mg/L)	*S* value cited in Howard (1989-1993).	2.50E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.46E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.44E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.19E-06
Log K_{ow} (unitless)	Hansch (1995).	1.79
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.75E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.75E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.31E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.12E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	6.17E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.48E+00
B	*B* value was obtained from U.S. EPA (1992b).	6.31E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.35E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-182

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPHENOL (88-75-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	3.5E+03

Note: NA = Not applicable, ND = No data available

TABLE A-1-183

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROPHENOL (100-02-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	139.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	386.1
Vp (atm)	*Vp* value cited in Howard (1989-1993).	1.32E-06 at 25°C (solid)
S (mg/L)	*S* value cited in Howard (1989-1993).	2.50E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	7.32E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.30E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.61E-06
Log K_{ow} (unitless)	Hansch (1995).	1.91
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.55E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.55E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.66E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	6.13E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	6.17E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.48E+00
B	*B* value was obtained from U.S. EPA (1992b).	8.13E-03

TABLE A-1-183

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROPHENOL (100-02-7)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.67E+01
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	NA
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	NA
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	8.28E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-184

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPROPANE (79-46-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	89.09
T_m (K)	U.S. EPA (1995g)	NA
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	2.40E-02
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.70E+05
H (atm·m^3/mol)	U.S. EPA (1995g)	1.23E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.23E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.01E-05
Log K_{ow} (unitless)	Chem. Inspect Test Inst. (1992).	0.93
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	6.53E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.53E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.90E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.30E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.10E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.30E-01
B	*B* value was obtained from U.S. EPA (1992b).	7.40E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.00E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-184

CHEMICAL-SPECIFIC INPUTS FOR 2-NITROPROPANE (79-46-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	Calculated from *RfC* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	5.71E-03
Oral CSF $(mg/kg/day)^{-1}$	Route to route extrapolation from Oral CSF.	9.4E+00
RfC (mg/m^3)	U.S. EPA (2004b)	2.00E-02
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	9.40E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-185

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROQUINOLINE-1-OXIDE (56-57-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	190.16
T_m (K)	CRC Handbook (1995)	427.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	8.00E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	1.09
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.40E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	NA
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-185

CHEMICAL-SPECIFIC INPUTS FOR 4-NITROQUINOLINE-1-OXIDE (56-57-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-186

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSODIETHYLAMINE (55-18-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	102.14
T_m (K)	--	
Vp (atm)	U.S. EPA (1995g)	2.60E-03
S (mg/L)	U.S. EPA (1995g)	2.00E+05
H (atm·m^3/mol)	U.S. EPA (1995g)	3.63E-06
D_a (cm^2/s)	U.S. EPA (1995g)	8.00E-02
D_w (cm^2/s)	U.S. EPA (1995g)	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	0.48
K_{oc} (mL/g)	U.S. EPA (1995g)	3.00E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.00E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.10E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	9.90E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.70E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.80E-01
B	*B* value was obtained from U.S. EPA (1992b).	3.00E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1995g)	6.30E-01
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-186

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSODIETHYLAMINE (55-18-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	1.52E+02
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	1.52E+02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-187

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSODIMETHYLAMINE (62-75-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	74.08
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	7.10E-03
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.00E+06
H (atm·m^3/mol)	U.S. EPA (1995g)	5.30-E07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	-0.57
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.24E-01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.24E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.18E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.70E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.90E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.70E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.17E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-187

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSODIMETHYLAMINE (62-75-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004c)	8.0E-06
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	5.10E+01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	4.90E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-188

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSO-DI-N-BUTYLAMINE (924-16-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	*MW* value cited in U.S. EPA (1995g)	158.20
T_m (K)	--	NA
Vp (atm)	*Vp* value cited in U.S. EPA (1995g)	3.80E-04 at 25°C
S (mg/L)	*S* value cited in U.S. EPA (1995g)	1.10E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.47E-05
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	6.50E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	7.52E-06
Log K_{ow} (unitless)	Hansch (1995).	2.63
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.45E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.45E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.09E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.10E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	8.10E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.90E+00
B	*B* value was obtained from U.S. EPA (1992b).	2.60E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	5.87E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-188

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSO-DI-N-BUTYLAMINE (924-16-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	5.4E+00
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	5.6E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-189

CHEMICAL-SPECIFIC INPUTS FOR NITROSO-DI-N-PROPYLAMINE, N- (621-64-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	263.23
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	310.1
Vp (atm)	*Vp* value cited in U.S. EPA (1992a).	1.30E-08 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	5.00E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.84E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.87E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.43E-06
Log K_{ow} (unitless)	Hansch (1995).	1.36
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.17E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.17E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.63E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.40E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.50E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.50E+00
B	*B* value was obtained from U.S. EPA (1992b).	7.90E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	6.36E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-189

CHEMICAL-SPECIFIC INPUTS FOR NITROSO-DI-N-PROPYLAMINE, N- (621-64-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	7.0E+00
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	Route to route extrapolation from Oral CSF.	7.0E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-190

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPHENYLAMINE (86-30-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	198.23
T_m (K)	Montgomery and Welkom (1991)	339.6
Vp (atm)	*Vp* value cited in U.S. EPA (1998c).	1.32E-04 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	3.50E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.99E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.12E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.35E-06
Log K_{ow} (unitless)	Hansch (1995).	3.13
K_{oc} (mL/g)	Estimated value was obtained from U.S. EPA (1994c).	3.27E+02, for pH range of 4.9 to 8.0
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.27E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.45E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.10E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.40E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.80E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.40E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.41E+02
BAF_{fish} (L/kg, FW)	--	NA

TABLE A-1-190

CHEMICAL-SPECIFIC INPUTS FOR *N*-NITROSODIPHENYLAMINE (86-30-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	4.9E-03
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	4.9E-03
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	5.85E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-191

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOMETHYLETHYLAMINE (10595-95-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	88.13
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.00E-03
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.00E+05
H (atm·m^3/mol)	U.S. EPA (1995g)	8.90E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Vera (1992).	0.04
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.29E+00
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.29E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.66E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.50E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.00E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.20E-01
B	*B* value was obtained from U.S. EPA (1992b).	7.60E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	6.32E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-191

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOMETHYLETHYLAMINE (10595-95-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	2.20E+01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	2.20E+01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-192

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOMORPHOLINE (59-89-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	116.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	302.15
Vp (atm)	--	NA
S (mg/L)	--	NA
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.00E-05
Log K_{ow} (unitless)	Hansch (1995).	-0.44
K_{oc} (mL/g)	--	NA
Kd_s (cm^3/g)	--	NA
Kd_{sw} (L/Kg)	--	NA
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.10E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.60E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-192

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOMORPHOLINE (59-89-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-193

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOPIPERIDINE (100-75-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	114.5
T_m (K)	--	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.90E-04
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.50E+05
H (atm·m^3/mol)	U.S. EPA (1995g)	1.40E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	0.36
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.31E+00
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.31E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.73E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.40E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	4.30E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.12E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-193

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOPIPERIDINE (100-75-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	CalEPA (1992)	9.4E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-194

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOPYRROLIDINE (930-55-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	100.11
T_m (K)	--	
Vp (atm)	*Vp* value cited in Montgomery and Weldom (1991).	2.30E-04
S (mg/L)	*S* value cited in U.S. EPA (1995g).	7.80E+05
H (atm·m^3/mol)	U.S. EPA (1995g)	2.90E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.36E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.04E-05
Log K_{ow} (unitless)	Hansch (1995).	-0.19
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	6.50E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.50E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.90E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.40E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.60E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.60E-01
B	*B* value was obtained from U.S. EPA (1992b).	6.50E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	4.22E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-194

CHEMICAL-SPECIFIC INPUTS FOR N-NITROSOPYRROLIDINE (930-55-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	2.10E+00
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	U.S. EPA (2004b)	2.14E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-195

CHEMICAL-SPECIFIC INPUTS FOR OCTAMETHYLPYROPHOSPHORAMIDE (152-16-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	286.26
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.30E-06
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.00E+06
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	3.80E-10
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.62E-06
Log K_{ow} (unitless)	K_{ow} value cited in U.S. EPA (1995g).	-0.52
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	3.10E-01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.10E-03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.30E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.50E-05
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.90E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.20E+01
B	*B* value was obtained from U.S. EPA (1992b).	3.00E-05
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.37E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-195

CHEMICAL-SPECIFIC INPUTS FOR OCTAMETHYLPYROPHOSPHORAMIDE (152-16-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	2.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.00E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-196

CHEMICAL-SPECIFIC INPUTS FOR PARATHION (ETHYL) (56-38-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	291.27
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.30E-08
S (mg/L)	*S* value cited in U.S. EPA (1995g).	6.50E+00
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	5.70E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.70E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.79E-06
Log K_{ow} (unitless)	Hansch (1995).	3.83
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	5.80E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.80E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.35E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.70E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	5.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	3.90E+01
B	*B* value was obtained from U.S. EPA (1992b).	6.80E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	BCFs were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	4.80E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-196

CHEMICAL-SPECIFIC INPUTS FOR PARATHION (ETHYL) (56-38-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	6.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	1.3E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1-197

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROBENZENE (608-93-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	250.34
T_m (K)	Montgomery and Welkom (1991)	358.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994f)	3.10E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994f)	3.20E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.43E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.86E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.34E-06
Log K_{ow} (unitless)	Hansch (1995).	5.17
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	3.21E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.21E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.40E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	3.10E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.90E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.40E+01
B	*B* value was obtained from U.S. EPA (1992b).	1.80E+01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	3.61E+04

TABLE A-1-197

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROBENZENE (608-93-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	8.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	US. EPA (1995f)	5.0E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-198

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROETHANE (76-01-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	202.31
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	244.15
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.815E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.60E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.30E-06
Log K_{ow} (unitless)	Hansch (1995).	3.22
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.63E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.50E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.05E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.12E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-198

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROETHANE (76-01-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2008)	9.0E-02
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-199

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	295.36
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	417.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994f). U.S. EPA (1994c) cites value from Howard (1989-1993)	3.10E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994f); U.S. EPA (1994c) cites value from Howard, Boethling, Jarvis, Meylan, and Michalenko (1991).	3.20E-02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt, (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	2.86E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	1.87E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	5.0E-06
Log K_{ow} (unitless)	Sangster (1994).	4.64
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.66E+03
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.66E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.24E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.90E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	5.50E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.80E+01
B	*B* value was obtained from U.S. EPA (1992b).	4.40E+00

TABLE A-1-199

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLORONITROBENZENE (82-68-8)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	4.65E+02
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.03E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	2.6E-01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-200

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	266.35
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	463
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	7.11E-07 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.34E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW, S* and *Vp* values that are provided in this table.	1.41E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	1.56E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database, U.S. EPA (1994d).	8.01E-06
Log K_{ow} (unitless)	Hansch (1995).	5.12
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c). The default value used in DRAS is based on a neutral pH.	pH / K_{oc} 1 19,949 2 19,918 3 19,604 4 16,942 5 7,333 6 1,417 7 504.9 8 408.7 9 399.1 10-14 398.1
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table. The default value used in DRAS is based on a neutral pH.	pH / K_{oc} 1 199.5 2 199.2 3 196.0 4 169.4 5 73.33 6 14.17 7 5.05 8 4.09 9 3.99 10-14 3.98
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} at a neutral pH that is provided in this table.	4.44E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.90E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.70E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.80E+01
B	*B* value was obtained from U.S. EPA (1992b).	1.20E+01

TABLE A-1-200

CHEMICAL-SPECIFIC INPUTS FOR PENTACHLOROPHENOL (87-86-5)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	3.97E+02
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.0E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.2E-01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	1E-03
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	1.5E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-201

CHEMICAL-SPECIFIC INPUTS FOR PHENACETIN (62-44-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	179.21
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	407.15 to 408.15
Vp (atm)	--	ND
S (g/1310ml of H_2O)	*S* value cited in U.S. EPA (1995b).	1.0
H (atm·m^3/mol)	H value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.41E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.70E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.82E-06
Log K_{ow} (unitless)	Nakagawa (1992).	1.58
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.03E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.08E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.60E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.80E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-201

CHEMICAL-SPECIFIC INPUTS FOR PHENACETIN (62-44-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-202

CHEMICAL-SPECIFIC INPUTS FOR PHENANTHRENE (85-01-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	178.22
T_m (K)	Montgomery and Welkom (1991)	371.1
Vp (atm)	Geometric mean value calculated from values cited in Montgomery and Welkom (1991).	1.35E-03 at 25°C (solid)
S (mg/L)	*S* value cited in Lucius et al. (1992).	1.28E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.88E-01
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.33E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.47E-06
Log K_{ow} (unitless)	Hansch (1995).	4.46
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.42E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.42E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.82E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.30E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.10E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.60E+00
B	*B* value was obtained from U.S. EPA (1992b).	2.90E+00

TABLE A-1-202

CHEMICAL-SPECIFIC INPUTS FOR PHENANTHRENE (85-01-8)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	Default *BAF* value recommended for use by U.S. EPA (1995g), when literature data were not available.	3.30E+03
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	NA
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	NA
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-203

CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	94.11
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	314.0
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	5.74E-04 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	9.08E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.95E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.27E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.03E-05
Log K_{ow} (unitless)	Hansch (1995).	1.46
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c). The default value in DRAS corresponds with a neutral pH.	pH / K_{oc} 1-7 22.0 8 21.8 9 20.0 10 11.2 11 2.27 12 0.51 13 0.32 14 0.30
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.20E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.65E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.70E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.30E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.90E-01
B	*B* value was obtained from U.S. EPA (1992b).	3.00E-03

TABLE A-1-203

CHEMICAL-SPECIFIC INPUTS FOR PHENOL (108-95-2)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	7.58E+00
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	2.56E-01

Note: NA = Not applicable, ND = No data available

TABLE A-1-204

CHEMICAL-SPECIFIC INPUTS FOR PHENOL MERCURIC ACETATE (62-38-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	130.19
T_m (K)	--	ND
Vp (atm)	Geometric mean value cited in U.S. EPA (1998c).	4.63E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1998c).	1.46E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.13E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.67E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.75E-06
Log K_{ow} (unitless)	Hansch (1995).	0.71
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.99E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.99E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.74E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	3.00E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	5.40E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.30E+00
B	*B* value was obtained from U.S. EPA (1992b).	2.50E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.04E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-204

CHEMICAL-SPECIFIC INPUTS FOR PHENOL MERCURIC ACETATE (62-38-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	8.0E-05
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)		ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-205

CHEMICAL-SPECIFIC INPUTS FOR 1,3-PHENYLENEDIAMINE (108-45-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	108.6
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	3.00E-05
S (mg/L)	*S* value cited in U.S. EPA (1995g).	3.50E+05
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	9.20E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.63E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.88E-06
Log K_{ow} (unitless)	Hansch (1995).	-0.33
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	1.10E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.10E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	8.25E-02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.50E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.00E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	9.60E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.10E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	U.S. EPA (1995g)	2.90E-01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-205

CHEMICAL-SPECIFIC INPUTS FOR 1,3-PHENYLENEDIAMINE (108-45-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	6.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-206

CHEMICAL-SPECIFIC INPUTS FOR PHORATE (298-02-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	260.4
T_m (K)	--	ND
Vp (atm)	*Vp* value cited in Montgomery and Welkom (1991).	1.70E-06 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	3.80E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.16E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.05E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.88E-06
Log K_{ow} (unitless)	Hansch (1995).	3.56
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.16E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.16E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.37E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	2.50E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.40E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	6.50E-01

TABLE A-1-206

CHEMICAL-SPECIFIC INPUTS FOR PHORATE (298-02-2)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.99E+02
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	2.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-207

CHEMICAL-SPECIFIC INPUTS FOR A-PICOLINE (109-06-8)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	93.12
T_m (°K)	--	203.15
Vp (mm@°C)	*Vp* value cited in U.S. EPA (1995g).	8.00E+00
S (mg/L)	*S* value cited in U.S. EPA (1995g).	
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	4.10E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.50E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.60E-06
Log K_{ow} (unitless)	Hansch (1995).	1.11
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	1.50E+06
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.50E+04
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.12E+05
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.16E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.24E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.76E-01
B	*B* value was obtained from U.S. EPA (1992b).	1.29E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-207

CHEMICAL-SPECIFIC INPUTS FOR A-PICOLINE (109-06-8)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-208

CHEMICAL-SPECIFIC INPUTS FOR POLYCHLORINATED BIPHENYLS (AROCLORS) (1336-36-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	328
T_m (°K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.00E-07
S (mg/L)	*S* value cited in U.S. EPA (1995g).	8.00E-02
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	2.60E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.00E-05
Log K_{ow} (unitless)	Hansch (1995).	6.29
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1998c).	9.83E+04
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.83E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.37E+03
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.30E+00
ô (hr)	ô value was obtained from U.S. EPA (1992b).	5.30E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.50E+01
B	*B* value was obtained from U.S. EPA (1992b).	3.20E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	The BAF_{fish} for PCBs was calculated by multiplying the composite total baseline BAF_{lipids} for trophic level 4 fish from 62 FR 11723, March 12, 1997 (5.27E+07) by the sample-weighted mean lipid content for trophic Level 4 fish (13.19%) cited in Table 2, Appendix 1 in U.S. EPA (1995e).	6.95E+06

TABLE A-1-208

CHEMICAL-SPECIFIC INPUTS FOR POLYCHLORINATED BIPHENYLS (AROCLORS) (1336-36-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b) Based on *high-risk* Aroclors,(i.e. Aroclor 1254)	2.0E-05
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	2.00E+00
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	7.0E-05
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	2.00E+00
MCL	National Primary Drinking Water Regulations.	5E-04
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	1.4E-02

Note: NA = Not applicable, ND = No data available

TABLE A-1-209

CHEMICAL-SPECIFIC INPUTS FOR PRONAMIDE (23950-58-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	256.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	428.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995g)	5.30E-07 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995g)	1.50E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	9.05E-06
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	4.71E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	5.45E-06
Log K_{ow} (unitless)	Ellington (1988).	3.43
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.35E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.35E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.77E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.60E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.70E+01
B	*B* value was obtained from U.S. EPA (1992b).	3.20E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.38E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-209

CHEMICAL-SPECIFIC INPUTS FOR PRONAMIDE (23950-58-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	7.5E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	2.6E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-210

CHEMICAL-SPECIFIC INPUTS FOR PYRENE (129-00-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	202.24
T_m (K)	Montgomery and Welkom (1991)	429.1
Vp (atm)	*Vp* value cited in U.S. EPA (1998c).	5.59E-09 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1992a).	1.30E-01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.14E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.72E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.14E-06
Log K_{ow} (unitless)	Hansch (1995).	4.88
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	6.80E+04
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	6.80E+02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.10E+03
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	4.70E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.50E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.20E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.30E+01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	8.73E+03

TABLE A-1-210

CHEMICAL-SPECIFIC INPUTS FOR PYRENE (129-00-0)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.05E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-211

CHEMICAL-SPECIFIC INPUTS FOR PYRIDINE (110-86-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	79.10
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	231.5
Vp (atm)	*Vp* value cited in U.S. EPA (1995g)	2.60E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g)	3.00E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.86E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.10E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.08E-05
Log K_{ow} (unitless)	Hansch (1995).	0.65
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	3.92E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.92E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.94E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.90E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.70E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	6.40E-01
B	*B* value was obtained from U.S. EPA (1992b).	4.70E-04
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.84E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-211

CHEMICAL-SPECIFIC INPUTS FOR PYRIDINE (110-86-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.0E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-212

CHEMICAL-SPECIFIC INPUTS FOR SAFROLE (94-59-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	162.18
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	284.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.10E-04 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.50E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.19E-05
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	4.06E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	7.16E-06
Log K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995).	2.66
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.12E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.12E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.09E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.50E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	8.50E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.00E+00
B	*B* value was obtained from U.S. EPA (1992b).	4.60E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	6.19E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-212

CHEMICAL-SPECIFIC INPUTS FOR SAFROLE (94-59-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-213

CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	78.96
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	490.1
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.03E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.20E-05
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)		NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. The default value in DRAS is based on a neutral pH.	18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). The default value in DRAS is based on a neutral pH.	18 at pH=4.9; 5.0 at pH=6.8; 2.2 at pH=8.0
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b).	1.29E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-213

CHEMICAL-SPECIFIC INPUTS FOR SELENIUM (7782-49-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.0E-03
Oral *CSF* $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation *CSF* $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	5E-02
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	5.0E+00

Note: NA = Not applicable, ND = No data available

TABLE A-1-214

CHEMICAL-SPECIFIC INPUTS FOR SILVER (7440-22-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	107.87
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	1,233.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	8.38E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	9.71E-06
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996a), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model. The default value in DRAS is based on a neutral pH.	0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). The default value in DRAS is based on a neutral pH.	0.1 at pH=4.9; 8.3 at pH=6.8; 110 at pH=8.0
Dermal Exposure Factors		
K_p^w (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b).	8.77E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-214

CHEMICAL-SPECIFIC INPUTS FOR SILVER (7440-22-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.0E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	1.2E-04

Note: NA = Not applicable, ND = No data available

TABLE A-1-215

CHEMICAL-SPECIFIC INPUTS FOR STRYCHNINE (57-24-9)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	334.40
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	541.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	2.20E-13 at 25°C (solid)
S (mg/L)	Montgomery and Welkom (1991)	1.50E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.90E-13
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.38E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.58E-06
Log K_{ow} (unitless)	Hansch (1995).	1.93
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.90E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.90E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.92E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	4.10E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	9.60E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.30E+01
B	*B* value was obtained from U.S. EPA (1992b).	8.50E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.73E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-215

CHEMICAL-SPECIFIC INPUTS FOR STRYCHNINE (57-24-9)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Note applicable, ND = No data available

TABLE A-1-216

CHEMICAL-SPECIFIC INPUTS FOR STYRENE (100-42-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	104.14
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	242.5
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	8.21E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	2.57E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.33E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.73E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.77E-06
Log K_{ow} (unitless)	Hansch (1995).	2.95
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	9.12E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.12E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	6.84E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.40E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.80E-01
t(hr/event)*	t* value was obtained from U.S. EPA (1992b).	9.10E-01
B	*B* value was obtained from U.S. EPA (1992b).	8.70E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.03E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-216

CHEMICAL-SPECIFIC INPUTS FOR STYRENE (100-42-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	1.02E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	1E-01
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-217

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4,5-TETRACHLOROBENZENE (95-94-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	215.89
T_m (K)	Montgomery and Welkom (1991)	411.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	7.1E-06 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.30E+00
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.18E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.11E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.75E-06
Log K_{ow} (unitless)	Hansch (1995).	4.64
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	5.66E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.66E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.24E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.80E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.80E+00
*t** (hr/event)	t* value was obtained from U.S. EPA (1992b).	9.10E+00
B	*B* value was obtained from U.S. EPA (1992b).	4.40E+00

TABLE A-1-217

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4,5-TETRACHLOROBENZENE (95-94-3)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	4.30E+03
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.0E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	5.0E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-218

CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8 -TETRACHLORODIBENZO (P) DIOXIN (1746-01-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1994a)	321.98
T_m (K)	U.S. EPA (1994a)	578.1
Vp (atm)	U.S. EPA (1994a)	9.74E-13 at 25°C (solid)
S (mg/L)	U.S. EPA (1994a)	1.93E-05
H (atm·m^3/mol)	U.S. EPA (1994a)	1.60E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.27E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.81E-06
Log K_{ow} (unitless)	Shiu (1998).	6.8
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for dioxins and furans that is cited in U.S. EPA (1994a; 1994b). Recommended value was calculated by using the recommended K_{ow} value that is provided in this table.	2.91E+05
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.91E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.18E+04
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.40E+00
ô (hr)	ô value was obtained from U.S. EPA (1992b).	8.10E+00
*t** (hr/event)	t* value was obtained from U.S. EPA (1992b).	3.80E+01
B	*B* value was obtained from U.S. EPA (1992b).	6.30E+02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg $_{FW\ tissue}$)	--	NA
BAF_{fish} (L/kg FW)	The BAF_{fish} for dioxin was calculated by multiplying the composite total baseline BAF_{lipids} for trophic level 4 fish from Table 10 in U.S. EPA (1995e) (9.0E+06) by the sample-weighted mean lipid content for trophic Level 4 fish (13.19%) cited in Table 2, Appendix 1 in U.S. EPA (1995e).	1.19E+06

TABLE A-1-218

CHEMICAL-SPECIFIC INPUTS FOR 2,3,7,8 -TETRACHLORODIBENZO (P) DIOXIN (1746-01-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	1.5E+05
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	1.5E+05
MCL	National Primary Drinking Water Regulations.	3.0E-08
Aquatic TRV (ug/l)	U.S. EPA (1995f)	1.0 E-08

Note: NA = Not Applicable, ND = No Data Available

TABLE A-1-219

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1,2-TETRACHLOROETHANE (630-20-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	167.85
T_m (K)	Montgomery and Welkom (1991)	230.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995g)	1.60E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g)	1.10E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.44E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.15E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.30E-06
Log K_{ow} (unitless)	Arithmetic mean value cited in Karickhoff and Long (1995)	2.63
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.45E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.45E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.09E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.30E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	9.20E-01
*t** (hr/event)	t* value was obtained from U.S. EPA (1992b).	2.20E+00
B	*B* value was obtained from U.S. EPA (1992b).	4.30E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	5.87E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-219

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1,2-TETRACHLOROETHANE (630-20-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.0E-02
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	2.6E-02
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	2.6E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-220

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2,2-TETRACHLOROETHANE (79-34-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	167.86
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	229.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	6.80E-03 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	3.07E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.72E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.16E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.26E-06
Log K_{ow} (unitless)	Hansch (1995).	2.39
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	7.90E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.90E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.92E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	9.00E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	9.20E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.20E+00
B	*B* value was obtained from U.S. EPA (1992b).	2.50E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.86E+01
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with a geometric mean of various laboratory measured *BCF*s obtained from various experimental studies cited in U.S. EPA (1998). *FCM*s were obtained from U.S. EPA (1995g)	4.33E+03

TABLE A-1-220

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2,2-TETRACHLOROETHANE (79-34-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2008)	4.0E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	2.0E-01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	2.0E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1996c)	4.2E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-221

CHEMICAL-SPECIFIC INPUTS FOR TETRACHLOROETHYLENE (127-18-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	165.85
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	251.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	2.42E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	2.32E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.73E-02
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	7.20E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	8.20E-06
Log K_{ow} (unitless)	Hansch (1995).	3.4
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.65E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.65E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.99E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.50E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	9.00E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.20E+00
B	*B* value was obtained from U.S. EPA (1992b).	4.70E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.26E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-221

CHEMICAL-SPECIFIC INPUTS FOR TETRACHLOROETHYLENE (127-18-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.0E-02
Oral CSF $(mg/kg/day)^{-1}$	CalEPA (2002) and CalEPA (2001)	5.4E-01
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	3.5E-02
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2002) and CalEPA (2001)	2.1E-02
MCL	National Primary Drinking Water Regulations.	5E-03
Aquatic TRV (ug/l)	U.S. EPA (1996c)	1.2E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-222

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	U.S. EPA (1995g)	231.89
T_m (K)	U.S. EPA (1995g)	343.0
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	6.60E-06 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.00E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from, Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.53E-05
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	2.55E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	5.78E-06
Log K_{ow} (unitless)	Hansch (1995).	4.45
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c). The default value in DRAS is based on a neutral pH.	pH / K_{oc} 1 6,190 2 6,188 3 6,166 4 5,956 5 4,456 6 1,323 7 249.2 8 115.3 9 101.6 10 100.2 11-14 100.0
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table for a *pH* of 7.0.	2.49
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.87E+01
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	8.30E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.30E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.30E+01
B	*B* value was obtained from U.S. EPA (1992b).	2.00E+00

TABLE A-1-222

CHEMICAL-SPECIFIC INPUTS FOR 2,3,4,6-TETRACHLOROPHENOL (58-90-2)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	2.51E+03
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.05E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-223

CHEMICAL-SPECIFIC INPUTS FOR TETRAETHYL DITHIOPYROPHOSPHATE (SULFOTEP) (3689-24-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	322.31
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	3.30E-07
S (mg/L)	*S* value cited in U.S. EPA (1995g).	2.50E+01
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	4.20E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Tomlin (1994).	3.99
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	5.80E+03
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	5.80E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	4.35E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	8.10E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	6.00E+01
B	*B* value was obtained from U.S. EPA (1992b).	6.80E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1995g)	2.80E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-223

CHEMICAL-SPECIFIC INPUTS FOR TETRAETHYL DITHIOPYROPHOSPHATE (SULFOTEP) (3689-24-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.00E-04
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.75E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-224

CHEMICAL-SPECIFIC INPUTS FOR THALLIUM (7440-28-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	204.38
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	576.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water.	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	5.48E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	6.34E-06
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	U.S. EPA (1996a). The default value in DRAS is based on a neutral pH.	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e). The default value in DRAS is based on a neutral pH.	44 at pH=4.9; 71 at pH=6.8; 96 at pH=8.0
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	--	ND
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b).	1.00E+04
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-224

CHEMICAL-SPECIFIC INPUTS FOR THALLIUM (7440-28-0)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	6.6E-05
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	2E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	4.00E+00

Note: NA = Not applicable, ND = No data available

TABLE A-1-225

CHEMICAL-SPECIFIC INPUTS FOR THIONAZIN (297-97-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	248.26
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	271.45
Vp (mmHg)	U.S. EPA (1995g)	3.00E-03
S (mg/L)	--	ND
H (atm·m^3/mol)	*H* value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.60E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	U.S. EPA (2000).	1.86
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.86E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-225

CHEMICAL-SPECIFIC INPUTS FOR THIONAZIN (297-97-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-226

CHEMICAL-SPECIFIC INPUTS FOR TIN (7440-31-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	118.69
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	505.05
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	--	ND
K_{oc} (mL/g)	--	ND
Kd_s (cm^3/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	ND
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-226

CHEMICAL-SPECIFIC INPUTS FOR TIN (7440-31-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	6.00E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	2.10E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-227

CHEMICAL-SPECIFIC INPUTS FOR TOLUENE (108-88-3)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	92.13
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	178.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	3.71E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	5.58E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	6.13E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.72E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.23E-06
Log K_{ow} (unitless)	Hansch (1995).	2.73
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.40E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.40E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.05E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	4.70E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.20E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	7.70E-01
B	*B* value was obtained from U.S. EPA (1992b).	5.60E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	7.00E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-227

CHEMICAL-SPECIFIC INPUTS FOR TOLUENE (108-88-3)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2005b)	8.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2005b)	5.0E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	1
Aquatic TRV (ug/l)	U.S. EPA (1996c)	1.3E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-228

CHEMICAL-SPECIFIC INPUTS FOR 2,4-TOLUENEDIAMINE (95-80-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	122.17
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.10E-07
S (mg/L)	*S* value cited in U.S. EPA (1995g).	7.50E+03
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	7.92E-10
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.05E-06
Log K_{ow} (unitless)	Debnath (1992).	0.14
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	2.50E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.50E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.88E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	6.60E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	4.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.20E+00
B	*B* value was obtained from U.S. EPA (1992b).	2.50E-04
Biotransfer Factors for Animals		
BCF_{fish} (unitless FW tissue)	U.S. EPA (1995g)	4.60E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-228

CHEMICAL-SPECIFIC INPUTS FOR 2,4-TOLUENEDIAMINE (95-80-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF (mg/kg/day)$^{-1}$	U.S. EPA (1997c)	3.20E+00
RfC (mg/m^3)	--	ND
Inhalation CSF (mg/kg/day)$^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	3.20E+00
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-229

CHEMICAL-SPECIFIC INPUTS FOR O-TOLUIDINE (95-53-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	107.15
T_m (K)	Montgomery and Welkom (1991)	258.4
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	3.94E-04 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.74E+04
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.43E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.14E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.12E-06
Log K_{ow} (unitless)	Hansch (1995).	1.32
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.99E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.99E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.49E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	3.80E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	9.50E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.20E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	5.93E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-229

CHEMICAL-SPECIFIC INPUTS FOR O-TOLUIDINE (95-53-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	NA
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	2.4E-01
RfC (mg/m^3)	--	NA
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-230

CHEMICAL-SPECIFIC INPUTS FOR P-TOLUIDINE (106-49-0)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	107.15
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	317.65
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	4.30E-04
S (mg/L)	*S* value cited in U.S. EPA (1995g).	7.60E+03
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	6.10E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	6.97E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.43E-06
Log K_{ow} (unitless)	Hansch (1995).	1.39
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	2.40E+01
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.40E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.80E+00
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.20E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	9.50E-01
B	*B* value was obtained from U.S. EPA (1992b).	2.50E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1995g)	3.50E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-230

CHEMICAL-SPECIFIC INPUTS FOR P-TOLUIDINE (106-49-0)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.90E-01
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	1.90E-01
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-231

CHEMICAL-SPECIFIC INPUTS FOR TOXAPHENE (CHLORINATED CAMPHENES) (8001-35-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	414
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	350.65
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	4.30E-04
S (mg/L)	*S* value cited in U.S. EPA (1995g).	6.79E-01
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	3.40E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.16E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.34E-06
Log K_{ow} (unitless)	Fisk (1999).	5.78
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	2.60E+05
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.60E+03
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.95E+04
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	4.60E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.90E+01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.40E+02
B	*B* value was obtained from U.S. EPA (1992b).	3.20E+01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	(U.S. EPA 1995g)	2.10E+06

TABLE A-1-231

CHEMICAL-SPECIFIC INPUTS FOR TOXAPHENE (CHLORINATED CAMPHENES) (8001-35-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.10E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	Value based on *Oral CSF* assuming route-to-route extrapolation.	1.10E+00
MCL	National Primary Drinking Water Regulations.	3E-03
Aquatic TRV (µg/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	2E-04

Note: NA = Not applicable, ND = No data available

TABLE A-1-232

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4-TRICHLOROBENZENE (120-82-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	181.46
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	290.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	4.42E-04 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	3.07E+01
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	2.61E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.23E-06
Log K_{ow} (unitless)	Hansch (1995).	4.02
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.66E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.66E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.24E+02
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.00E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.10E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	9.50E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.00E+00
Biotransfer Factors for Animals (Continued)		
BCF_{fish} (L/kg $_{\text{FW tissue}}$)	--	NA

TABLE A-1-232

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4-TRICHLOROBENZENE (120-82-1)

Parameter	Reference and Explanation	Value
BAF_{fish} (L/kg FW)	*BAF*s were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	8.79E+02

TABLE A-1-232

CHEMICAL-SPECIFIC INPUTS FOR 1,2,4-TRICHLOROBENZENE (120-82-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004c)	3.5E-03
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	7E-02
Aquatic TRV (ug/l)	U.S. EPA (1996c)	1.11E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-233

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1-TRICHLOROETHANE (71-55-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	133.42
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	242.7
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c)	1.63E-01 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c)	1.17E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.86E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.64E+02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.56E-06
Log K_{ow} (unitless)	Hansch (1995).	2.49
K_{oc} (mL/g)	Geometric mean value cited in U.S. EPA (1996b)	1.35E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.35E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.01E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.10E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	8.70E-02
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.10E-01
B	*B* value was obtained from U.S. EPA (1992b).	3.00E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	4.60E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-233

CHEMICAL-SPECIFIC INPUTS FOR 1,1,1-TRICHLOROETHANE (71-55-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2007b)	2.0E+00
Oral CSF $(mg/kg/day)^{-1}$	--	NA
RfC (mg/m^3)	U.S. EPA (2007b)	5.0E+00
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	2E-01
Aquatic TRV (ug/l)	U.S. EPA (1995f)	5.28E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-234

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLOROETHANE (79-00-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	133.42
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	238.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.31E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	4.40E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.00E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.51E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.0E-05
Log K_{ow} (unitless)	Hansch (1995).	1.89
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	7.50E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.50E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.62E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	8.30E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	5.70E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.40E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.10E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.61E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-234

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLOROETHANE (79-00-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	4.0E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	5.70E-02
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	5.6E-02
MCL	National Primary Drinking Water Regulations.	5E-03
Aquatic TRV (ug/l)	U.S. EPA (1995f)	9.40E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-235

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROETHYLENE (79-01-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	131.40
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	188.3
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	9.48E-02 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	1.18E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.06E-02
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.65E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.94E-06
Log K_{ow} (unitless)	Hansch (1995).	2.42
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.88E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.88E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.41E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.60E-01
ô (hr)	ô value was obtained from U.S. EPA (1992b).	8.70E-02
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	2.10E-01
B	*B* value was obtained from U.S. EPA (1992b).	5.10E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	4.07E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-235

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROETHYLENE (79-01-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2001c) Note: this value is provisional	3.0E-04
Oral CSF $(mg/kg/day)^{-1}$	CalEPA (2002)	1.3E-02
RfC (mg/m^3)	CalEPA (2000a)	6.0E-01
Inhalation CSF $(mg/kg/day)^{-1}$	CalEPA (2002)	7.0E-03
MCL	National Primary Drinking Water Regulations.	5E-03
Aquatic TRV (ug/l)	U.S. EPA (1996c)	3.5E+02

Note: NA = Not applicable, ND = No data available

TABLE A-1-236

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE (76-13-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	187.38
T_m (°K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	4.80E-01
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.70E+02
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	4.815E-01
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.80E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.20E-06
Log K_{ow} (unitless)	Hansch (1995).	3.16
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	1.30E+03
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.30E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.81E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	2.40E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.10E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.40E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.48E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-236

CHEMICAL-SPECIFIC INPUTS FOR 1,1,2-TRICHLORO-1,2,2-TRIFLUOROETHANE (76-13-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.00E+01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (1997c)	3.0E+01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-237

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROFLUOROMETHANE (75-69-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	137.38
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	162.1
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.10E+00 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.10E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	1.37E-01
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	4.27E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.0E-05
Log K_{ow} (unitless)	Hansch (1995).	2.53
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.21E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.21E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.06E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.70E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	6.00E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.40E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.40E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	4.93E+01
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-237

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROFLUOROMETHANE (75-69-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (1997c)	7.0E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-238

CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOL (95-95-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	197.46
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	340.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	2.15E-05 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.53E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	5.64E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.91E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.03E-06
Log K_{ow} (unitless)	Hansch (1995).	3.72
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c). The default value used in DRAS is based on a neutral pH.	pH / K_{oc} 1-3 / 2,380 4 / 2,377 5 / 2,353 6 / 2,139 7 / 1,127 8 / 223.7 9 / 56.14 10 / 37.94 11 / 36.10 12 / 35.92 13-14 / 35.90
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. The default value used in DRAS is based on a neutral pH.	1.60E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.20E+02
Dermal Exposure Factors		
K_p^w (cm/hr)	K_p^w value was obtained from U.S. EPA (1992b).	7.00E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.40E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.10E+01
B	*B* value was obtained from U.S. EPA (1992b).	7.90E-01

TABLE A-1-238

CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOL (95-95-4)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.96E+02
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-239

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	197.46
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	342.1
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	1.55E-05 at 25°C (solid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.53E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	4.06E-06
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.62E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.08E-06
Log K_{ow} (unitless)	Hansch (1995).	3.69
K_{oc} (mL/g)	For all ionizing organics, K_{oc} values were estimated on the basis of pH. Estimated values were obtained from U.S. EPA (1994c). The default value used in DRAS is based on a neutral pH.	pH / K_{oc} 1 / 1,070 2 / 1,070 3 / 1,069 4 / 1,063 5 / 1,006 6 / 670.8 7 / 226.2 8 / 120.4 9 / 108.4 10 / 107.1 11-14 / 107.0
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. The default value used in DRAS is based on a neutral pH.	3.81E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.86E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	5.00E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.40E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	9.20E+00
B	*B* value was obtained from U.S. EPA (1992b).	5.00E-01

TABLE A-1-239

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6-TRICHLOROPHENOL (88-06-2)

Parameter	Reference and Explanation	Value
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.75E+02
BAF_{fish} (L/kg FW)	--	NA
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2007c)	1.0E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.1E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	3.5E-04
Inhalation CSF $(mg/kg/day)^{-1}$	U.S.EPA (2004b)	1.1E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	U.S. EPA (1995f)	3.2E+00

Note: NA = Not applicable, ND = No data available

TABLE A-1-240

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROPHENOXY PROPIONIC ACID (SILVEX) (93-72-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	269.51
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	6.80E-09
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.40E+02
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	1.30E-08
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	3.8
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	2.30E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.30E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.71E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.10E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.90E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.90E+01
B	*B* value was obtained from U.S. EPA (1992b).	2.60E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	4.55E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-240

CHEMICAL-SPECIFIC INPUTS FOR TRICHLOROPHENOXY PROPIONIC ACID (SILVEX) (93-72-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	8.00E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	2.80E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	5E-02
Aquatic TRV (µg/l)	--.	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-241

CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOXYACETIC ACID (93-76-5)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	255.49
T_m (K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	9.10E-10
S (mg/L)	*S* value cited in U.S. EPA (1995g).	2.80E+02
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	8.68E-09
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.00E-06
Log K_{ow} (unitless)	Hansch (1995).	3.31
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	1.80E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.80E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.35E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.20E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.20E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.30E+01
B	*B* value was obtained from U.S. EPA (1992b).	2.00E-01
Biotransfer Factors for Animals		
BCF_{fish} (unitless FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.93E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-241

CHEMICAL-SPECIFIC INPUTS FOR 2,4,5-TRICHLOROPHENOXYACETIC ACID (93-76-5)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	1.00E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	3.50E-02
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-242

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROPROPANE (96-18-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Montgomery and Welkom (1991)	147.43
T_m (K)	Montgomery and Welkom (1991)	258.4
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	4.90E-03 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.90E+03
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.80E-04
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.99E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.24E-06
Log K_{ow} (unitless)	Chem Inspect Test Inst. (1992).	2.27
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	7.52E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	7.52E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	5.64E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	9.50E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	6.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.70E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.80E-02
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	3.13E+01
BAF_{fish} (L/kg FW	--	NA

TABLE A-1-242

CHEMICAL-SPECIFIC INPUTS FOR 1,2,3-TRICHLOROPROPANE (96-18-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	6.0E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (1997c)	7.0E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-243

CHEMICAL-SPECIFIC INPUTS FOR O,O,O-TRIETHYLPHOSPHOROTHIATE (126-68-1)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	CRC Handbook (1995)	198.22
T_m (°K)	--	ND
Vp (atm)	--	ND
S (mg/L)	--	ND
H (atm·m^3/mol)	--	ND
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	3.17E-02
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	6.23E-06
Log K_{ow} (unitless)	U.S. EPA (2000).	2.64
K_{oc} (mL/g)	--	ND
Kd_s (mL/g)	--	ND
Kd_{sw} (L/Kg)	--	ND
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	ND
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.42E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	ND
B	*B* value was obtained from U.S. EPA (1992b).	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	ND
BAF_{fish} (L/kg FW)	--	ND

TABLE A-1-243

CHEMICAL-SPECIFIC INPUTS FOR O,O,O-TRIETHYLPHOSPHOROTHIATE (126-68-1)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (water) (mg/kg/day)	--	ND
RfD (food) (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-244

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRINITROBENZENE (99-35-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neill, Smith, and Heckelman (1989)	213.11
T_m (K)	Budavari, O'Neill, Smith, and Heckelman (1989)	395.6
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.30E-07 at 25°C (solid)
S (mg/L)	*S* value cited in U.S. EPA (1995g).	3.20E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	8.66E-08
D_a (cm^2/s)	D_a value was obtained from WATER8 model database (U.S. EPA 1995d).	2.84E-02
D_w (cm^2/s)	D_w value was obtained from WATER8 model database (U.S. EPA 1995d).	6.08E-06
Log K_{ow} (unitless)	Hansch (1995).	1.18
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	1.03E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.03E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.73E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	6.57E-04
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.75E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.19E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.51E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	4.64E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-244

CHEMICAL-SPECIFIC INPUTS FOR 1,3,5-TRINITROBENZENE (99-35-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.0E-02
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-245

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6 -TRINITROTOLUENE (118-96-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	227.13
T_m (K)	Montgomery and Welkom (1991)	353.2
Vp (atm)	*Vp* value cited in U.S. EPA (1998c).	2.63E-07
S (mg/L)	*S* value cited in U.S. EPA (1998c).	1.30E+02
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1998c).	4.59E-07
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	2.62E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.85E-06
Log K_{ow} (unitless)	Hansch (1995).	1.6
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	2.22E+01
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.22E-01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.66E+00
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	1.31E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.75E+00
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	4.19E+00
B	*B* value was obtained from U.S. EPA (1992b).	3.98E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	9.68E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-245

CHEMICAL-SPECIFIC INPUTS FOR 2,4,6 -TRINITROTOLUENE (118-96-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	5.0E-04
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	3.0E-02
RfC (mg/m^3)	Calculated from *RfD* using an inhalation rate of 20 m^3/day and a human body weight of 70 kg.	1.75E-03
Inhalation CSF $(mg/kg/day)^{-1}$	Route to route extrapolation from Oral CSF.	3.0E-02
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-246

CHEMICAL-SPECIFIC INPUTS FOR TRIS(2,3-DIBROMOPROPYL) PHOSPHATE B19 (126-72-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	697.93
T_m (K)	--	ND
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	2.00E-07
S (mg/L)	*S* value cited in U.S. EPA (1995g).	4.70E+00
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	3.00E-05
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	5.50E-03
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	3.66E-06
Log K_{ow} (unitless)	Sangster (1994).	4.29
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	2.80E+03
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.80E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.10E+02
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	3.30E-05
ô (hr)	ô value was obtained from U.S. EPA (1992b).	1.60E+03
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	8.60E+03
B	*B* value was obtained from U.S. EPA (1992b).	3.20E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	*BAFs* were used for compounds with a log K_{ow} value above 4.0, as cited in U.S. EPA (1995g). *BAF* values were predicted values calculated by multiplying a food chain multiplier (*FCM*) with an estimated *BCF*. *BCF*s were estimated using the correlation equation obtained from Veith, Macek, Petrocelli, and Caroll (1980). *FCM*s were obtained from U.S. EPA (1995g)	1.60E+03

TABLE A-1-246

CHEMICAL-SPECIFIC INPUTS FOR TRIS(2,3-DIBROMOPROPYL) PHOSPHATE B19 (126-72-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	--	ND
Oral CSF $(mg/kg/day)^{-1}$	CalEPA (1992).	2.3E+00
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-247

CHEMICAL-SPECIFIC INPUTS FOR VANADIUM (7440-62-2)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	--	50.94
T_m (K)	--	
Vp (atm)	--	N/A
S (mg/L)	--	N/A
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	--	NA
D_w (cm^2/s)	--	NA
Log K_{ow} (unitless)	--	N/A
K_{oc} (mL/g)	--	N/A
Kd_s (cm^3/g)	U.S. EPA (1995g)	5.00E+01
Kd_{sw} (L/Kg)	--	5.00E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	--	NA
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-247

CHEMICAL-SPECIFIC INPUTS FOR VANADIUM (7440-62-2)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b) Value derived from the RfD for vanadium pentoxide.	5.04E-03
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1996c)	1.9E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-248

CHEMICAL-SPECIFIC INPUTS FOR VINYL ACETATE (108-05-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	--	50.94
T_m (K)	--	
Vp (atm)	--	N/A
S (mg/L)	--	N/A
H (atm·m^3/mol)	--	NA
D_a (cm^2/s)	--	NA
D_w (cm^2/s)	--	NA
Log K_{ow} (unitless)	Hansch (1995).	0.73
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for phthalates and PAHs, / all nonionizing organics except phthalates, PAHs, dioxins, and furans, cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	4.53E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	4.53E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	3.40E-01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	1.00E-03
ô (hr)	--	ND
t (hr/event)*	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	2.11E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-248

CHEMICAL-SPECIFIC INPUTS FOR VINYL ACETATE (108-05-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (1997c)	1.0E+00
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	2.0E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (µg/l)	U.S. EPA (1996c)	1.9E+01

Note: NA = Not applicable, ND = No data available

TABLE A-1-249

CHEMICAL-SPECIFIC INPUTS FOR VINYL CHLORIDE (75-01-4)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	62.50
T_m (K)	Budavari, O'Neil, Smith, and Heckelman (1989)	119.3
Vp (atm)	Geometric mean value cited in U.S. EPA (1994c).	3.68E+00 at 25°C (liquid)
S (mg/L)	Geometric mean value cited in U.S. EPA (1994c).	7.30E+02
H (atm·m^3/mol)	*H* value was calculated by using the theoretical equation from Lyman, Reehl, and Rosenblatt (1982), which defines the constant. Recommended value was calculated by using the *MW*, *S*, and *Vp* values that are provided in this table.	3.15E-01
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.58E-01
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	1.19E-05
Log K_{ow} (unitless)	Geometric mean value cited in U.S. EPA (1994c).	1.14
K_{oc} (mL/g)	K_{oc} value was calculated by using the correlation equation with K_{ow} for all nonionizing organics except phthalates, PAHs, dioxins, and furans as cited in U.S. EPA (1994c). K_{oc} value was calculated by using the recommended K_{ow} value that is provided in this table.	9.58E+00
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed fraction organic carbon of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	9.58E-02
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	7.18E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	9.20E-03
ô (hr)	ô value was obtained from U.S. EPA (1992b).	2.10E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	5.10E-01
B	*B* value was obtained from U.S. EPA (1992b).	3.20E-03
Biotransfer Factors for Animals		
BCF_{fish} (L/kg, FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	4.33E+00
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-249

CHEMICAL-SPECIFIC INPUTS FOR VINYL CHLORIDE (75-01-4)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.0E-03
Oral CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	1.4E+00
RfC (mg/m^3)	U.S. EPA (2004b)	1.0E-01
Inhalation CSF $(mg/kg/day)^{-1}$	U.S. EPA (2004b)	3.1E-02
MCL	National Primary Drinking Water Regulations.	2E-03
Aquatic TRV (ug/l)	--	ND

Note: NA = Not applicable, ND = No data available

TABLE A-1-250

CHEMICAL-SPECIFIC INPUTS FOR *M*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	106.16
T_m (K)	Montgomery and Welkom (1991)	225.7
Vp (atm)	*Vp* value cited in U.S. EPA (1998c).	1.06E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1998c).	1.86E+02
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1998c).	6.05E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.49E-06
Log K_{ow} (unitless)	Hansch (1995).	3.12
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	1.96E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.96E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.47E-01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	7.60E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.30E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.50E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.38E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-250

CHEMICAL-SPECIFIC INPUTS FOR *M*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	1.02E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	1.0E+01
Aquatic TRV (ug/l)	Suter (1996)	2.7E+03

Note: NA = Not applicable, ND = No data available

TABLE A-1-251

CHEMICAL-SPECIFIC INPUTS FOR *O*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	106.16
T_m (K)	Montgomery and Welkom (1991)	248.1
Vp (atm)	*Vp* value cited in U.S. EPA (1998c).	1.06E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1998c).	1.86E+02
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1998c).	6.05E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.69E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.44E-06
Log K_{ow} (unitless)	Hansch (1995).	3.12
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	2.41E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	2.41E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	1.80E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	7.60E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.30E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.50E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.38E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-251

CHEMICAL-SPECIFIC INPUTS FOR *O*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	1.02E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	1.0E+01
Aquatic TRV (ug/l)	Suter (1996)	2.7E+03

Note: NA = Not applicable, ND = No data available

TABLE A-1-252

CHEMICAL-SPECIFIC INPUTS FOR *P*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	106.16
T_m (K)	Montgomery and Welkom (1991)	286.1
Vp (atm)	*Vp* value cited in U.S. EPA (1998c).	1.06E-02 at 25°C (liquid)
S (mg/L)	*S* value cited in U.S. EPA (1998c).	1.86E+02
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1998c).	6.05E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.61E+02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	8.50E-06
Log K_{ow} (unitless)	Hansch (1995).	3.12
K_{oc} (mL/g)	Geometric mean of measured values obtained from U.S. EPA (1996b).	3.11E+02
Kd_s (cm^3/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	3.11E+00
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	2.33E+01
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	$K_p{}^w$ value was obtained from U.S. EPA (1992b).	7.60E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.30E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.50E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.38E+02
BAF_{fish} (L/kg FW)	--	NA

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CHEMICAL-SPECIFIC INPUTS FOR *P*-XYLENE (1330-20-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	1.02E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	1.0E+01
Aquatic TRV (ug/l)	Suter (1996)	2.7E+03

Note: NA = Not applicable, ND = No data available

TABLE A-1-253

CHEMICAL-SPECIFIC INPUTS FOR XYLENES (TOTAL) (1330-20-7)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	106.17
T_m (°K)	--	
Vp (atm)	*Vp* value cited in U.S. EPA (1995g).	1.10E-02
S (mg/L)	*S* value cited in U.S. EPA (1995g).	1.90E+02
H (atm·m^3/mol)	*H* value cited in U.S. EPA (1995g).	6.00E-03
D_a (cm^2/s)	D_a value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	7.14E-02
D_w (cm^2/s)	D_w value was obtained from CHEMDAT8 database (U.S. EPA 1994d).	9.34E-06
Log K_{ow} (unitless)	Hansch (1995).	3.12
K_{oc} (mL/g)	K_{oc} value cited in U.S. EPA (1995g).	1.30E+03
Kd_s (mL/g)	Kd_s value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.01 in soil. Measured organic carbon in soil, specific to site conditions, should be used to calculate Kd_s, because the value varies, depending on the fraction of organic carbon in soil. Recommended Kd_s value was calculated by using the K_{oc} value that is provided in this table.	1.30E+01
Kd_{sw} (L/Kg)	Kd_{sw} value was calculated by using the correlation equation with K_{oc} that is cited in U.S. EPA (1993) for an assumed organic carbon fraction of 0.075 in suspended sediment. Measured organic carbon in suspended sediment, specific to site conditions, should be used to calculate Kd_{sw}, because the value varies, depending on the fraction of organic carbon in suspended sediment. Recommended Kd_{sw} value was calculated by using the K_{oc} value that is provided in this table.	9.75E+01
Dermal Exposure Factors		
Kp (cm/hr)	*Kp* value was obtained from U.S. EPA (1992b).	7.60E-02
ô (hr)	ô value was obtained from U.S. EPA (1992b).	3.90E-01
t (hr/event)*	t* value was obtained from U.S. EPA (1992b).	1.30E+00
B	*B* value was obtained from U.S. EPA (1992b).	1.50E-01
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW)	*BCFs* were used for compounds with a log K_{ow} value below 4.0, as cited in U.S. EPA (1995g). BCF_{fish} value calculated using the correlation equation with K_{ow} obtained from Veith, Macek, Petrocelli, and Caroll (1980)	1.38E+02
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-253

CHEMICAL-SPECIFIC INPUTS FOR XYLENES (TOTAL) (1330-20-7)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	2.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	U.S. EPA (2004b)	1.02E-01
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	1.0E+01
Aquatic TRV (µg/l)	U.S. EPA (1996c)	1.80E+00

Note: Not applicable, ND = No data available

TABLE A-1-254

CHEMICAL-SPECIFIC INPUTS FOR ZINC (7440-66-6)

Parameter	Reference and Explanation	Value
Chemical/Physical Properties		
MW (g/mole)	Budavari, O'Neil, Smith, and Heckelman (1989)	65.38
T_m (°K)	Budavari, O'Neil, Smith, and Heckelman (1989)	692.6
Vp (atm)	All metals, except mercury, are assumed to be nonvolatile at ambient temperatures.	0.0
S (mg/L)	All metals, except mercury, are assumed to be insoluble in water. OR Budavari, O'Neil, Smith, and Heckelman (1989)	0.0
H (atm·m^3/mol)	*H* value is assumed to be zero, because the *Vp* and *S* values are zero for all metals, except mercury.	0.0
D_a (cm^2/s)	D_a value was calculated using the equation cited in U.S. EPA (1996a).	1.17E-01
D_w (cm^2/s)	D_w value was calculated using the equation cited in U.S. EPA (1996a).	1.36E-05
Log K_{ow} (unitless)	--	NA
K_{oc} (mL/g)	--	NA
Kd_s (mL/g)	Kd_s value was obtained from U.S. EPA (1996), which provides pH-based values that were estimated by using the MINTEQ2 geochemical speciation model.	6.2E+01 at pH=6.8
Kd_{sw} (L/Kg)	Kd_{sw} value is assumed to be the same as the Kd_s value, because organic carbon does not play a major role in sorption for the metals, as cited in US. EPA (1994e).	6.2E+01 at pH=6.8
Dermal Exposure Factors		
$K_p{}^w$ (cm/hr)	--	ND
ô (hr)	--	ND
t^* (hr/event)	--	ND
B	--	ND
Biotransfer Factors for Animals		
BCF_{fish} (L/kg FW tissue)	U.S. EPA (1998b).	2.06E+03
BAF_{fish} (L/kg FW)	--	NA

TABLE A-1-254

CHEMICAL-SPECIFIC INPUTS FOR ZINC (7440-66-6)

Parameter	Reference and Explanation	Value
Health Benchmarks		
RfD (mg/kg/day)	U.S. EPA (2004b)	3.0E-01
Oral CSF $(mg/kg/day)^{-1}$	--	ND
RfC (mg/m^3)	--	ND
Inhalation CSF $(mg/kg/day)^{-1}$	--	ND
MCL	National Primary Drinking Water Regulations.	ND
Aquatic TRV (ug/l)	Ambient Water Quality Criteria, U.S. EPA, Office of Water.	1.20E+02

Note: NA = Not applicable, ND = No data available

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CHEMICAL-SPECIFIC INPUTS FOR ZINC (7440-66-6)